

An entropic gradient structure for Lindblad equations and GENERIC for quantum systems coupled to macroscopic models*

Markus Mittnenzweig and Alexander Mielke
WIAS Berlin

19. September 2016

1 Introduction

In many situations the evolution of quantum systems is dictated not only by the system Hamiltonian but also by dissipative effects, i.e. the time-dependent density matrix $\rho(t)$ satisfies an evolution equation

$$\dot{\rho} = \frac{i}{\hbar} [\rho, H] + \mathcal{L}\rho, \quad (1.1)$$

where we will set $\hbar = 1$ in the sequel. The dissipative part \mathcal{L} of this Lindblad equation has to be a completely positive operator, which is enforced by the structure of quantum mechanics. In this work we additionally ask for the **condition of detailed balance**, see (2.5). Equations of this type were already derived in [Dav74] as the weak coupling limit of a given quantum system with a large heat bath. It was observed in [Spo78] that this class of models satisfies the detailed-balance condition (DBC) and that the relative entropy (also called free energy)

$$\mathcal{F}(\rho) = \text{Tr} \left(\rho (\log \rho - \log \hat{\rho}_\beta) \right) = \text{Tr} \left(\rho (\log \rho + \beta H) \right) + \log Z_\beta$$

is a Liapunov function, i.e. it decays along solutions. Here $\beta > 0$ is a suitable inverse temperature and

$$\hat{\rho}_\beta = \frac{1}{Z_\beta} e^{-\beta H} \quad \text{with } Z_\beta = \text{Tr} (e^{-\beta H})$$

is the thermal equilibrium.

The aim of this work is to show that (1.1) can be written as a damped Hamiltonian system, namely

$$\dot{\rho} = (\mathbb{J}(\rho) - \mathbb{K}(\rho)) D\mathcal{F}(\rho), \quad (1.2)$$

*Partially supported by ERC AdG 267802 AnaMultiScale and by the DFG via SFB 787 Nanophotonics (subproject B4).

where the operator $\mathbb{J}(\rho) : \xi \mapsto \frac{i}{\beta}[\rho, \xi]$ generates a Poisson bracket, while the operator $\mathbb{K}(\rho)$ should be purely dissipative, i.e. $\mathbb{K}(\rho) = \mathbb{K}(\rho)^* \geq 0$. We will call such dissipative operators simply ***Onsager operators***, because of Onsager's fundamental work in [Ons31].

Thus, our aim is the construction of an Onsager operator \mathbb{K} which generalizes the Wasserstein operator $\mathbb{K}_{\text{Wass}}(u) : \mu \mapsto -\text{div}(\rho \nabla \mu)$ for the Fokker-Planck equation and the Markov operator $\mathbb{K}_{\text{Mv}}(p)$ for jump processes constructed in [Mie11b, Maa11, ErM12, Mie13b], cf. Section 3.1. The crucial point is that $\mathbb{K}(\rho)$ has to depend on ρ in a very specific way to obtain the relation

$$-\mathbb{K}(\rho)(\log \rho + \beta H) = \mathcal{L}\rho,$$

where the right-hand side is linear in ρ . In the Fokker-Planck equation this is achieved by the chain rule $u \nabla (\log u + V) = \nabla u + u \nabla V$, and for jump processes it follows from $\Lambda(a, b)(\log a - \log b) = a - b$, see Section 3.1.

For quantum systems first steps in this direction were done in [Ött10, Ött11, Mie13a, CaM14, Mie15]. They involve the use of the Kubo-Mori operator

$$\mathfrak{C}_\rho : L(\mathbf{H}) \rightarrow L(\mathbf{H}); \quad A \mapsto \mathfrak{C}_\rho A := \int_0^1 \rho^s A \rho^{1-s} ds,$$

which satisfies for all $Q \in L(\mathbf{H})$ the fundamental relation

$$\mathfrak{C}_\rho [Q, \log \rho] = [Q, \rho], \quad (1.3)$$

which we will call the miracle relation. Obviously, we need a generalization allowing for commutators of the form $[Q, \log \rho + \beta H]$, which is nontrivial if $\beta H \neq \alpha \mathbf{1}_{\mathbf{H}}$. In [CaM14] the infinite-temperature case $\beta H = 0$ is treated, while in [Ött10, Ött11, Mie13a, Mie15] the nonlinear terms $\rho \mapsto \mathfrak{C}_\rho[Q, H]$ are admitted.

Here, we show that in the general case satisfying the DBC it is possible to find a suitable \mathbb{K} in a rather natural way. The starting point is a tensor-product representation of Lindblad operators. We set $\mathbf{H}_1 = \mathbf{H}$ and choose an arbitrary second Hilbert space \mathbf{H}_2 and assume that \mathbf{H}_1 and \mathbf{H}_2 are finite-dimensional. For an arbitrary Hermitian $\mathbb{Q} \in L(\mathbf{H}_1 \otimes \mathbf{H}_2)$ and a $\hat{\sigma} \in L(\mathbf{H}_2)$ with $\hat{\sigma} = \hat{\sigma}^* > 0$ one sees that

$$\mathcal{L}\rho = -\text{Tr}_{\mathbf{H}_2} \left([\mathbb{Q}, [\mathbb{Q}, \rho \otimes \hat{\sigma}]] \right) \quad (1.4)$$

is indeed a Lindblad operator. Moreover, it can be shown easily, that this \mathcal{L} satisfies the DBC with respect to $\hat{\rho}_\beta$ if the commutation relation

$$[\mathbb{Q}, \hat{\rho}_\beta \otimes \hat{\sigma}] = 0$$

holds, see Section 2.3. Under this condition it is now straightforward to show the following generalization of the miracle identity:

$$\mathfrak{C}_{\rho \otimes \hat{\sigma}} [\mathbb{Q}, (\log \rho + \beta H) \otimes \mathbf{1}_{\mathbf{H}_2}] = [\mathbb{Q}, \rho \otimes \hat{\sigma}].$$

Indeed, it suffices to use the fact that \mathbb{Q} also commutes with $\log(\hat{\rho}_\beta \otimes \hat{\sigma}) = -\beta H \otimes \mathbf{1}_{\mathbf{H}_2} + \mathbf{1}_{\mathbf{H}_1} \otimes \log \hat{\sigma}$ and then apply the classical miracle identity (1.3), see Theorem 3.4 for the details. Now we can define the Onsager operator

$$\mathbb{K}(\rho)\xi = \text{Tr}_{\mathbf{H}_2} \left([\mathbb{Q}, \mathfrak{C}_{\rho \otimes \hat{\sigma}}[\mathbb{Q}, \xi \otimes \mathbf{1}_{\mathbf{H}_2}]] \right), \quad (1.5)$$

which is a symmetric and positive semidefinite operator and satisfies the desired relation

$$-\mathbb{K}(\rho)(\log \rho + \beta H) = -\text{Tr}_{\mathbf{H}_2} \left([\mathbb{Q}, [\mathbb{Q}, \rho \otimes \hat{\sigma}]] \right) = \mathcal{L}\rho.$$

In Theorem 2.7 we show that every Lindblad operator satisfying the DBC with respect to $\hat{\rho}_\beta$ can be written in the form (1.4) with $\mathbf{H}_2 = \mathbf{H} = \mathbf{H}_1$ and either $\hat{\sigma} = \hat{\rho}_\beta$ or $\hat{\sigma} = \hat{\rho}_\beta^{-1}$. For this result we rely on the classical characterization of Lindblad operators satisfying the DBC in [Ali76, KF*77].

In Sections 4 and 5 we consider a few applications and discuss the general problem of modeling the interaction of a macroscopic system described by a state variable $z \in Z$. We show that it is possible to set up a coupled system in the framework of GENERIC, which is an acronym for “General Equations for Non-Equilibrium Reversible and Irreversible Coupling”. This framework is based on an energy functional \mathcal{E} , an entropy functional \mathcal{S} , a Poisson operator \mathbb{J} , and an Onsager operator \mathbb{K} such that the evolution is

$$\begin{pmatrix} \dot{\rho} \\ \dot{z} \end{pmatrix} = \mathbb{J}_{\text{coupl}}(\rho, z) \begin{pmatrix} D_\rho \mathcal{E}(\rho, z) \\ D_z \mathcal{E}(\rho, z) \end{pmatrix} + \mathbb{K}_{\text{coupl}}(\rho, z) \begin{pmatrix} D_\rho \mathcal{S}(\rho, z) \\ D_z \mathcal{S}(\rho, z) \end{pmatrix}.$$

This is complemented by the fundamental ***non-interaction conditions*** $\mathbb{J}D\mathcal{S} \equiv 0 \equiv \mathbb{K}D\mathcal{E}$ that defines a thermodynamically consistent system with energy conservation and entropy production. The typical choice for the functionals is

$$\mathcal{E}(\rho, z) = \text{Tr}(\rho H) + E(z) \quad \text{and} \quad \mathcal{S}(\rho, z) = -k_B \text{Tr}(\rho \log \rho) + S(z).$$

To describe the coupling of the quantum system with the variable z it is essential to model the different dissipation mechanisms separately, which we do by the minimal building blocks \mathbf{S}_W and $\mathbf{M}_{\beta, Q}$ for Lindblad operators, where Q must satisfy $[Q, H] = \omega Q$ for some $\omega \in R$. The associated Onsager operators $\mathbf{K}_{\beta, Q}$ can then be obtained from the construction (1.5) by choosing

$$\mathbb{Q} = Q^* \otimes \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + Q \otimes \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \quad \text{and} \quad \hat{\sigma} = \begin{pmatrix} e^{\beta\omega/2} & 0 \\ 0 & e^{-\beta\omega/2} \end{pmatrix}.$$

With the above choice for \mathcal{E} we have $D_\rho \mathcal{E}(\rho, z) = H$, which forces us to use fixed eigenpairs (ω, Q) . However, we may assume that the effective coupling temperature may depend on z and may differ for different coupling mechanisms. Hence, a typical Onsager operator for the coupled system may have the form

$$\mathbb{K}_{\text{coupl}}(\rho, z) = \sum_{m=1}^M \begin{pmatrix} \mathbf{K}_{\tilde{\beta}_m(z), Q_m}(\rho) & \langle \square, b_m(z) \rangle_Z \mathbf{K}_{\tilde{\beta}_m(z), Q_m}(\rho) H \\ \langle \mathbf{K}_{\tilde{\beta}_m(z), Q_m}(\rho) \square \mid H \rangle b_m(z) & \langle \mathbf{K}_{\tilde{\beta}_m(z), Q_m}(\rho) H \mid H \rangle b_m(z) \otimes b_m(z) \end{pmatrix}.$$

For an application to the thermodynamically consistent modeling of the Maxwell-Bloch system as considered in [JMR00, Dum05] we refer to Section 5.4, where the macroscopical variable $z = (\mathbf{E}, \mathbf{H})$ contains the electric and the magnetic field. For more applications, also involving the coupling to drift-diffusion equations we refer to [Mie15, Sec. 5].

2 Dissipative quantum mechanics

2.1 General notations and setup

Here we recall the standard theory and introduce our notation. The quantum mechanical system is described by states in a complex Hilbert space \mathbf{H} . For simplicity we only consider the finite-dimensional case $\mathbf{H} = \mathbb{C}^N$, but the main constructions can be extended to infinite dimensions if the convergence questions are suitably addressed.

We use the scalar product $\langle a|b \rangle = \sum_{j=1}^N \bar{a}_j b_j$. For a Hamiltonian operator $H \in \mathbb{C}_{\text{Herm}}^{N \times N}$ (the set of Hermitian matrices) the associated Hamiltonian dynamics is given via the Schrödinger equation

$$\dot{\psi} = -iH\psi, \quad (2.1)$$

which has the solution $\psi(t) = e^{-itH}\psi(0)$.

To couple a quantum system to a macroscopic one we need to describe it in terms of the multi-particle form using the density matrices

$$\rho \in \mathfrak{R}_N := \{ \rho \in \mathbb{C}^{N \times N} \mid \rho = \rho^* \geq 0, \text{Tr } \rho = 1 \}.$$

Hence, each $\rho \in \mathfrak{R}$ has the representation

$$\rho = \sum_{j=1}^N r_j \psi_j \otimes \bar{\psi}_j, \quad (2.2)$$

where $r_j \geq 0$, $\sum_1^N r_j = 1$, and $\{ \psi_j \mid j = 1, \dots, N \}$ is an orthonormal set. Note that in our notation $(\psi \otimes \bar{\phi})a := \langle \phi|a \rangle \psi$ and $(\psi \otimes \bar{\phi})A = \psi \otimes \overline{(A^* \phi)}$.

On operators we define the scalar product

$$\langle A \mid B \rangle = \text{Tr}(A^* B) = \sum_{j,k=1}^N \bar{A}_{jk} B_{jk}$$

This scalar product satisfies the following identities, which we will use without further notice below:

$$\begin{aligned} \langle A \mid B \rangle &= \langle B^* \mid A^* \rangle = \overline{\langle B \mid A \rangle}, & \langle \lambda A \mid \mu B \rangle &= \bar{\lambda} \mu \langle A \mid B \rangle, \\ \langle A \mid BC \rangle &= \langle AC^* \mid B \rangle = \langle B^* A \mid C \rangle, \\ \langle A \mid [B, C] \rangle &= \langle B^* \mid [C, A^*] \rangle = \langle C^* \mid [A^*, B] \rangle, \end{aligned}$$

where $\lambda, \mu \in \mathbb{C}$ and $A, B, C \in \mathbb{C}^{N \times N}$.

2.2 The Lindblad equations

Using (2.1) the evolution of ρ is given via the Liouville–von Neumann equation

$$\dot{\rho} = -i[H, \rho], \quad \text{where } [\rho, H] := \rho H - H \rho. \quad (2.3)$$

For open systems, dissipative versions of the Hamiltonian Liouville–von Neumann equation are used. The most general linear master equation preserving complete positivity is the Lindblad equation which is of the form

$$\dot{\rho} = -i[H, \rho] + \mathcal{L}\rho \quad \text{with } \mathcal{L}A = \sum_{n,m=1}^{N^2-1} a_{n,m}([Q_n, AQ_m^*] + [Q_n A, Q_m^*]), \quad (2.4)$$

where Q_n are arbitrary operators in $L(\mathbf{H}) := \text{Lin}(\mathbf{H}, \mathbf{H})$, and $(a_{n,m})$ forms a Hermitian positive semi-definite matrix. Note that \mathcal{L} in the Lindblad equation is only evaluated on $\rho = \rho^* \in \mathfrak{R}$, while we define \mathcal{L} as an operator mapping all of $L(\mathbf{H})$ into $L(\mathbf{H})$. It is easily seen that all these \mathcal{L} are $*$ -operators, i.e. they satisfy $\mathcal{L}(A^*) = (\mathcal{L}A)^*$. The set of all Lindblad operators forms a cone in the set of linear operators from $L(\mathbf{H})$ into itself, which has real dimension $(N^2-1)^2$.

We are mainly interested in Lindblad operators satisfying the detailed balance condition. Let \mathcal{L}^* denote the adjoint of \mathcal{L} defined via $\langle \mathcal{L}^*A | B \rangle = \langle A | \mathcal{L}B \rangle$. The **condition of detailed balance** with respect to the equilibrium state $\hat{\rho}_\beta$ is defined via the relation

$$\text{(DBC)} \quad \begin{cases} \mathcal{L}\hat{\rho}_\beta = 0, \\ \langle \mathcal{L}^*(A) | B\hat{\rho}_\beta \rangle = \langle A | \mathcal{L}^*(B)\hat{\rho}_\beta \rangle \quad \text{for all } A, B \in L(\mathbf{H}). \end{cases} \quad (2.5)$$

The characterization of all Lindblad operators lying in the class of operators satisfying the DBC for a fixed $\hat{\rho}_\beta$ is given in [Ali76, Eqn. (20)], and we will derive a new and compact representation of these operators in Section 2.3. Clearly, the DBC is equivalent to

$$\mathcal{L}(A\hat{\rho}_\beta) = \mathcal{L}^*(A)\hat{\rho}_\beta \quad \text{for all } A \in L(\mathbf{H}). \quad (2.6)$$

Before discussing the general form of **all** Lindblad operators satisfying the DBC, we will construct minimal building blocks, which are useful in their own right for the modeling of dissipative couplings as discussed in Sections 4 and 5. The main observation is that the property of detailed balance with respect to $\hat{\rho}_\beta = \frac{1}{Z_\beta}e^{-\beta H}$ involves operators Q having the property $\hat{\rho}_\beta Q(\hat{\rho}_\beta)^{-1} = \mu Q$, which can be characterized by the following elementary result.

Lemma 2.1 *For $\omega \in \mathbb{R}$, $H \in \mathbb{C}_{\text{Herm}}^{N \times N}$, and $Q \in \mathbb{C}^{N \times N}$ we have the equivalences:*

$$\begin{aligned} (i) \quad [Q, H] = \omega Q &\iff \exists (ii) \quad \beta \neq 0 : e^{-\beta H} Q e^{\beta H} = e^{\beta \omega} Q \\ &\iff (iii) \quad \forall \gamma \in \mathbb{R} : e^{-\gamma H} Q e^{\gamma H} = e^{\gamma \omega} Q. \end{aligned} \quad (2.7)$$

We note that operators with the commutator property (i) can easily be constructed when using the spectral representation of the Hamiltonian H , namely

$$H = \sum_{n=1}^N \varepsilon_n h_n \otimes \overline{h_n}, \quad \text{and hence } \hat{\rho}_\beta = \frac{1}{Z_\beta} \sum_{n=1}^N e^{-\beta \varepsilon_n} h_n \otimes \overline{h_n} \text{ with } Z_\beta = \sum_{n=1}^N e^{-\beta \varepsilon_n}.$$

For a given eigenvalue ε_n we define the spectral projector P_n via

$$P_n = \sum_{k: \varepsilon_k = \varepsilon_n} h_k \otimes \overline{h_k}, \quad \text{giving } P_n = P_n^2 = P_n^* \text{ and } P_n H = H P_n = \varepsilon_n P_n.$$

Now we can take any operator $V \in \mathbb{C}^{N \times N}$ and choose spectral projectors P_n and P_m , then

$$Q = P_n V P_m \quad \text{satisfies} \quad [Q, H] = (\varepsilon_m - \varepsilon_n)Q.$$

We emphasize that this relation is linear in Q , so that a general Q satisfying $[Q, H] = \omega Q$ may have the form

$$Q = \sum_{(n,m): \varepsilon_m - \varepsilon_n = \omega} P_n V_{n,m} P_m,$$

thus possibly more than two energy levels ε_k may be involved. This is trivial for the case $\omega = 0$ but may also occur in the case $\omega \neq 0$. See Example 2.4.2.

We introduce the spectrum $\Omega(H)$ of $A \mapsto [A, H]$ and the set $\mathfrak{E}(H)$ of eigenpairs vis

$$\begin{aligned} \Omega(H) &:= \text{spec}([\cdot, H]) = \{ \varepsilon_m - \varepsilon_n \mid \varepsilon_n, \varepsilon_m \in \text{spec}(H) \}, \\ \mathfrak{E}(H) &:= \{ (\omega, Q) \in \mathbb{R} \times \mathbb{C}^{N \times N} \mid [Q, H] = \omega Q \}. \end{aligned}$$

Let us further define the multiplicities of the eigenspaces via

$$d_\omega = \dim \{ Q \in \mathbb{C}^{N \times N} \mid [Q, H] = \omega Q \}.$$

If H has only one-dimensional eigenspaces and no pairs of eigenvalues $\varepsilon_m, \varepsilon_n$ ($m \neq n$) have equal differences $\varepsilon_m - \varepsilon_n = \varepsilon_{m'} - \varepsilon_{n'}$, then $d_\omega = 1$ for $\omega \neq 0$ and $d_0 = N$. In the most degenerate case $H = 0$ we have $d_0 = N^2$. The following result provides the building blocks for all Lindblad operators satisfying the detailed balance condition with respect to $\hat{\rho}_\beta = \frac{1}{Z_\beta} e^{-\beta H}$.

Proposition 2.2 (Building blocks \mathbf{S}_W and $\mathbf{M}_{\beta, Q}$) *Let H and $\hat{\rho}_\beta$ be given as above.*

(a) *Consider any $W \in \mathbb{C}_{\text{Herm}}^{N \times N}$ with $[W, H] = 0$, then the operator \mathbf{S}_W defined by*

$$\mathbf{S}_W A := [W, AW] + [WA, W] = [W, [A, W]]$$

is a Lindblad operator satisfying $\mathbf{S}_W = \mathbf{S}_W^$ and the DBC for $\hat{\rho}_\beta$.*

(b) *Consider any pair $(\omega, Q) \in \mathfrak{E}(H)$, then the operator $\mathbf{M}_{\beta, Q}$ defined via*

$$\mathbf{M}_{\beta, Q} A := e^{\beta\omega/2} ([Q, AQ^*] + [QA, Q^*]) + e^{-\beta\omega/2} ([Q^*, AQ] + [Q^* A, Q])$$

is a Lindblad operator satisfying the DBC for $\hat{\rho}_\beta$.

(c) *Every Lindblad operator \mathcal{L} satisfying the DBC (2.5) can be written in the form*

$$\mathcal{L} = \sum_{j=1}^J \mathbf{S}_{W_j} + \sum_{m=1}^M \mathbf{M}_{\beta, Q_m}, \quad \text{where} \quad \begin{cases} W_j = W_j^*, \quad (0, W_j) \in \mathfrak{E}(H), \text{ and} \\ (\omega_m, Q_m) \in \mathfrak{E}(H) \text{ with } \omega_m > 0. \end{cases}$$

The numbers J and M of necessary terms is bounded by $J \leq d_0 - 1$ and $M \leq \sum_{\omega \in \Omega(H) \setminus \{0\}} d_\omega$.

Proof. Part (a): Obviously, \mathbf{S}_W is a special case of \mathcal{L} in (2.4) by choosing $a_{1,1} = 1$ and $Q_1 = W$ and $a_{n,m} = 0$ for $(n, m) \neq (1, 1)$, so it is a Lindblad operator. We also see that the DBC $\mathbf{S}_W^{\hat{\rho}_\beta} = \mathbf{S}_W$ holds, since $\hat{\rho}_\beta W \hat{\rho}_\beta^{-1} = W$ by using Lemma 2.1.

Part (b): It is obvious that $\mathbf{M}_{\beta,Q}$ has the form of \mathcal{L} in (2.4) with $Q_1 = Q$, $Q_2 = Q^*$, $a_{1,1} = e^{\beta\omega/2}$, and $a_{2,2} = e^{-\beta\omega/2}$, while all other terms are 0. Moreover, $\mathbf{M}_{\beta,Q}^{\hat{\rho}_\beta}$ can be calculated explicitly by using Lemma 2.1 and $\hat{\rho}_\beta Q^* \hat{\rho}_\beta^{-1} = e^{-\beta\omega} Q^*$, so the DBC follows.

Part (c): From [KF*77, Eqn. (2.16)-(2.20)] (where L_s corresponds to our \mathcal{L}^*) we know that every Lindblad operator satisfying the DBC with respect to $\hat{\rho}_\beta$ can be written as

$$\mathcal{L}A = \sum_{k,j=1}^N D_{kj} ([X_{kj}A, X_{kj}^*] + [X_{kj}, AX_{kj}^*]), \quad (2.8)$$

where $D_{kj} \geq 0$ and $X_{kj} \in \mathbb{C}^{N \times N}$ satisfy the conditions (with $\hat{r}_j = e^{-\beta\varepsilon_j}/Z_\beta > 0$)

$$\begin{aligned} & \text{(i) } D_{kj}\hat{r}_j = D_{jk}\hat{r}_k \text{ and } X_{kj}^* = X_{jk} \text{ for } \hat{r}_j \neq \hat{r}_k; \quad \text{(ii) } \langle X_{kj} | X_{lm} \rangle = \delta_{kl}\delta_{jm}; \\ & \text{(iii) } X_{kj}^* = X_{kj} \text{ for } \hat{r}_j = \hat{r}_k; \quad \text{(iv) } \hat{\rho}_\beta X_{kj} (\hat{\rho}_\beta)^{-1} = \frac{\hat{r}_k}{\hat{r}_j} X_{kj}. \end{aligned} \quad (2.9)$$

We decompose the set $I = \{1, \dots, N\}^2$ into $I_\neq := \{(k, j) \in \{1, \dots, N\}^2 \mid \hat{r}_j \neq \hat{r}_k\}$ and $I_ = := \{(k, j) \in \{1, \dots, N\}^2 \mid \hat{r}_j = \hat{r}_k\}$. For $(j, k) \in I_\neq$ the second condition in (i) gives $X_{jk} = X_{kj}^*$, while (iv) and Lemma 2.1 imply $(\varepsilon_k - \varepsilon_j, X_{kj}) \in \mathfrak{E}(H)$. Using now the first condition in (i) as well and setting $Q_{kj} = e^{\beta(\varepsilon_k - \varepsilon_j)/4} X_{kj}$, we find the relation

$$D_{kj} ([X_{kj}A, X_{kj}^*] + [X_{kj}, AX_{kj}^*]) + D_{jk} ([X_{jk}A, X_{jk}^*] + [X_{jk}, AX_{jk}^*]) = \mathbf{M}_{\beta, Q_{kj}} A.$$

For $(k, j) \in I_ =$ conditions (iii) and (iv) yield $X_{kj} = X_{kj}^*$ and $[X_{kj}, H] = 0$. Thus,

$$D_{kj} ([X_{kj}A, X_{kj}^*] + [X_{kj}, AX_{kj}^*]) = \mathbf{S}_{W_{kj}} A \text{ with } W_{kj} = \sqrt{D_{kj}} X_{kj}.$$

In summary, we find that \mathcal{L} in (2.8) can be written in the form

$$\mathcal{L} = \sum_{(k,j) \in I_ =} \mathbf{S}_{W_{kj}} + \sum_{(k,j) \in I_\neq, j < k} \mathbf{M}_{\beta, Q_{kj}},$$

which is the desired result. ■

Note that the representation of \mathcal{L} in terms of the Kraus operators Q_n in (2.4) is not unique. Correspondingly, our representation in terms of \mathbf{S}_{W_j} and \mathbf{M}_{Q_j} is not unique. Moreover, for a minimal representation one may ask for additional orthogonality conditions. We also remark that the operators \mathbf{S}_W can be obtained from \mathbf{M}_Q as a special case allowing $\omega = 0$ and asking for $Q = Q^*$. More precisely, if $(0, Q) \in \mathfrak{E}(H)$ then also $(0, Q^*)$ and $(0, \frac{1}{2}(Q + Q^*))$ lie in $\mathfrak{E}(H)$. In particular, we have

$$(0, Q) \in \mathfrak{E}(H) \text{ and } Q = Q^* \implies \mathbf{M}_{\beta, Q} = 2\mathbf{S}_{\beta, Q} = \mathbf{S}_{\beta, \sqrt{2}Q}.$$

Moreover, $(\omega, Q) \in \mathfrak{E}(H)$ if and only if $(-\omega, Q^*) \in \mathfrak{E}(H)$ and $\mathbf{M}_{\beta, Q} = \mathbf{M}_{\beta, Q^*}$. Thus, Proposition 2.2(c) tells us that all Lindblad operators satisfying the DBC can be written in the form

$$\mathcal{L}\rho = \sum_{n=1}^N \mathbf{M}_{\beta, Q_n} \rho \quad \text{where } (\omega_n, Q_n) \in \mathfrak{E}(H) \text{ and } \omega_j \in \Omega(H). \quad (2.10)$$

We will see specific examples in Sections 2.4 and 5. The above representation in terms of the building blocks is especially useful for modeling, while the next section provides a form that is more elegant and compact.

2.3 A compact form of all DBC Lindblad operators

In this section we will write Lindblad operators and our building blocks 2.2 in another way. The basic idea is to write them as the partial trace of a double commutator on a larger space. This will prove useful in Section 3 when writing down entropic gradient structures for the Lindblad equations with DBC. In what follows \mathbf{H}_1 and \mathbf{H}_2 denote finite-dimensional Hilbert spaces, and for $A \in L(\mathbf{H}_1)$ and $B \in L(\mathbf{H}_2)$ we denote the tensor product by $A \otimes B \in L(\mathbf{H}_1) \otimes L(\mathbf{H}_2) = L(\mathbf{H}_1 \otimes \mathbf{H}_2)$. We also introduce the notion of a partial trace

$$\text{Tr}_{\mathbf{H}_2} : L(\mathbf{H}_1) \otimes L(\mathbf{H}_2) \rightarrow L(\mathbf{H}_1) \text{ defined via } \text{Tr}_{\mathbf{H}_2}(A \otimes B) = \text{Tr}_2(B)A$$

and by linearity, where Tr_2 is the trace in $L(\mathbf{H}_2)$.

The next result shows that all Lindblad operators on $L(\mathbf{H}_1)$ can be written in a compact form by a double commutator on $L(\mathbf{H}_1) \otimes L(\mathbf{H}_2)$ and a partial trace. Moreover, this form allows for a simple criterion for the DBC with respect to the equilibrium $\hat{\rho}_\beta$.

Proposition 2.3 (Compact representation for \mathcal{L}) *Consider two finite-dimensional Hilbert spaces \mathbf{H}_1 and \mathbf{H}_2 . Assume that $\mathbb{Q} \in L(\mathbf{H}_1) \otimes L(\mathbf{H}_2)$ and $\hat{\sigma} \in L(\mathbf{H}_2)$ are Hermitian and $\hat{\sigma} \geq 0$, then*

$$\mathcal{L}(\rho) = -\text{Tr}_{\mathbf{H}_2} \left([\mathbb{Q}, [\mathbb{Q}, \rho \otimes \hat{\sigma}]] \right) \quad (2.11)$$

is a Lindblad operator in $L(\mathbf{H}_1)$, i.e. the generator of a completely positive semigroup.

If in addition \mathbb{Q} and $\hat{\sigma}$ satisfy the commutator relation

$$[\mathbb{Q}, \hat{\rho}_\beta \otimes \hat{\sigma}] = 0, \quad (2.12)$$

then \mathcal{L} satisfies the DBC with respect to $\hat{\rho}_\beta$.

Proof. Since $\hat{\sigma} \geq 0$ we can write $\hat{\sigma} = \sum_{j=1}^J \sigma_j e_j \otimes \bar{e}_j$ with $\sigma_j \geq 0$. Let us define

$$Q_{kl} = \langle e_k | \mathbb{Q} | e_l \rangle_{\mathbf{H}_2} = \text{Tr}_{\mathbf{H}_2}(\mathbf{1}_{\mathbf{H}_1} \otimes (e_l \otimes \bar{e}_k) \mathbb{Q}) \text{ giving } \mathbb{Q} = \sum_{k,l} Q_{kl} \otimes (e_l \otimes \bar{e}_k).$$

Then $Q_{kl} = Q_{lk}^*$ and using $\text{Tr}_{\mathbf{H}_2}(B \otimes ((e_k \otimes \bar{e}_l) \otimes (e_m \otimes \bar{e}_n))) = \delta_{kn} \delta_{lm} B$ we find

$$\mathcal{L}\rho = \sum_{k,l=1}^J (2\sigma_l Q_{kl} \rho Q_{lk} - \sigma_k \{Q_{kl} Q_{lk}, \rho\}) = \sum_{k,l=1}^J \sigma_l ([Q_{kl} \rho, Q_{kl}^*] + [Q_{kl}, \rho Q_{kl}^*]). \quad (2.13)$$

which is clearly of Lindblad form.

The commutation relation (2.12) immediately implies $\mathcal{L}\hat{\rho}_\beta = 0$, which is the first relation in the DBC (2.5). The second relation is written in terms of the dual operator \mathcal{L}^* that takes the form

$$\mathcal{L}^*(A) = \text{Tr}_{\mathbf{H}_2}(\mathbf{1}_{\mathbf{H}_1} \otimes \hat{\sigma} [\mathbb{Q}, [\mathbb{Q}, A \otimes \mathbf{1}_{\mathbf{H}_2}]]).$$

We have to show $\text{Tr}((\mathcal{L}^*A)^*B\hat{\rho}_\beta) = \text{Tr}(A^*\mathcal{L}^*(B)\hat{\rho}_\beta)$ which, upon using $(\mathcal{L}^*A)^* = \mathcal{L}^*(A^*)$, is equivalent to

$$\begin{aligned}\text{Tr}_{\mathbf{H}_1}(\mathcal{L}^*(A^*)B\hat{\rho}_\beta) &= \text{Tr}_{\mathbf{H}_1 \otimes \mathbf{H}_2}(\mathbf{1}_{\mathbf{H}_1} \otimes \hat{\sigma} [\mathbb{Q}, [\mathbb{Q}, A^* \otimes \mathbf{1}_{\mathbf{H}_2}]] (B\hat{\rho}_\beta) \otimes \mathbf{1}_{\mathbf{H}_2}) \\ &= \text{Tr}_{\mathbf{H}_1 \otimes \mathbf{H}_2}([\mathbb{Q}, [\mathbb{Q}, A^* \otimes \mathbf{1}_{\mathbf{H}_2}]] (B \otimes \mathbf{1}_{\mathbf{H}_2}) \hat{\rho}_\beta \otimes \hat{\sigma}).\end{aligned}$$

Again using the commutator condition (2.12) we obtain, for all \mathbb{A} , the identity

$$[\mathbb{Q}, \mathbb{A}(\hat{\rho}_\beta \otimes \hat{\sigma})] = +[\mathbb{Q}, \mathbb{A}] \hat{\rho}_\beta \otimes \hat{\sigma} + \mathbb{A} [\mathbb{Q}, \hat{\rho}_\beta \otimes \hat{\sigma}] = [\mathbb{Q}, \mathbb{A}] \hat{\rho}_\beta \otimes \hat{\sigma},$$

which we use twice, namely once with $\mathbb{A} = B \otimes \mathbf{1}_{\mathbf{H}_2}$ and once with $\mathbb{A} = [\mathbb{Q}, B \otimes \mathbf{1}_{\mathbf{H}_2}]$. Thus, we can move the \mathbb{Q} operators to the right and obtain

$$\begin{aligned}\text{Tr}_{\mathbf{H}_1}(\mathcal{L}^*(A^*)B\hat{\rho}_\beta) &= \text{Tr}_{\mathbf{H}_1 \otimes \mathbf{H}_2}(A^* \otimes \mathbf{1}_{\mathbf{H}_2} [\mathbb{Q}, [\mathbb{Q}, (B \otimes \mathbf{1}_{\mathbf{H}_2})]] \hat{\rho}_\beta \otimes \hat{\sigma}) \\ &= \text{Tr}_{\mathbf{H}_1}(A^* \text{Tr}_{\mathbf{H}_2}([\mathbb{Q}, [\mathbb{Q}, (B \otimes \mathbf{1}_{\mathbf{H}_2})]] \mathbf{1} \otimes \hat{\sigma}) \hat{\rho}_\beta) \\ &= \text{Tr}_{\mathbf{H}_1}(A^* \mathcal{L}^*(B) \hat{\rho}_\beta),\end{aligned}$$

which is the desired DBC. ■

The above result shows that the commutator relation (2.12) is crucial for the study of Lindblad operators satisfying the DBC. In the following lemma we give an alternative characterization which will be useful later, when studying the associated gradient structures.

Lemma 2.4 (Equivalent commutation relation) *Consider $\mathbb{Q} = \mathbb{Q}^* \in L(\mathbf{H}_1) \otimes L(\mathbf{H}_2)$, $\hat{\rho} \in L(\mathbf{H}_1)$, and $\hat{\sigma} \in L(\mathbf{H}_2)$ with $\hat{\rho} = \hat{\rho}^* > 0$ and $\hat{\sigma} = \hat{\sigma}^* > 0$. Then, we have*

$$[\mathbb{Q}, \hat{\rho} \otimes \hat{\sigma}] = 0 \iff [\mathbb{Q}, \log \hat{\rho} \otimes \mathbf{1}_{\mathbf{H}_2}] + [\mathbb{Q}, \mathbf{1}_{\mathbf{H}_1} \otimes \log \hat{\sigma}] = 0. \quad (2.14)$$

Proof. We simply note that a Hermitian operator \mathbb{Q} commutes with a Hermitian operator $\mathbb{B} > 0$ if and only if it commutes with its logarithm $\log \mathbb{B}$. We apply this to $\mathbb{B} = \hat{\rho} \otimes \hat{\sigma}$, for which we have

$$\log(\hat{\rho} \otimes \hat{\sigma}) = \log \hat{\rho} \otimes \mathbf{1}_{\mathbf{H}_2} + \mathbf{1}_{\mathbf{H}_1} \otimes \log \hat{\sigma}.$$

This gives the desired result. ■

The above proposition shows that the definition (2.11) together with (2.12) generates Lindblad operators satisfying the DBC. Obviously the building block $\mathbf{S}_W A = [W, [A, W]]$ does also fall into that class since it is already in double commutator form and $[W, H] = 0$. The following corollary shows that the building blocks \mathbf{S}_W and $\mathbf{M}_{\beta, Q}$ from Proposition 2.2 can be written in the compact form (2.11) as well.

Corollary 2.5 (Building blocks from compact form) *For $H = H^* \in L(\mathbf{H}_1)$ consider $\hat{\rho}_\beta = \frac{1}{Z_\beta} e^{-\beta H}$.*

(1) *Choosing $\mathbf{H}_2 = \mathbb{C}$ and $\mathbb{Q}_W = W$ for $W = W^* \in L(\mathbf{H}_1)$ we have the identity*

$$\mathbf{S}_W A = [W, AW] + [WA, W] = -[W, [W, A]] = -[\mathbb{Q}_W, [\mathbb{Q}_W, A]].$$

The commutator relation (2.14) for \mathbb{Q}_W is simply $[H, W] = 0$.

(2) Choosing $\mathbf{H}_2 = \mathbb{C}^2$ and $(\omega, Q) \in \mathfrak{E}(H)$ we define

$$\mathbb{Q}_Q = \begin{pmatrix} 0 & Q^* \\ Q & 0 \end{pmatrix} \quad \hat{\sigma}_{\beta\omega} = \begin{pmatrix} e^{\beta\omega/2} & 0 \\ 0 & e^{-\beta\omega/2} \end{pmatrix}.$$

Then, the commutation relation (2.14) holds and we have

$$\begin{aligned} \mathbf{M}_{\beta,Q} A &= -\text{Tr}_{\mathbf{H}_2}([\mathbb{Q}_Q, [Q_Q, A \otimes \hat{\sigma}_{\beta\omega}]]) \\ &= e^{\beta\omega/2}([Q, \rho Q^*] + [Q\rho, Q^*]) + e^{-\beta\omega/2}([Q^*, \rho Q] + [Q^*\rho, Q]). \end{aligned} \quad (2.15)$$

Proof. (1) is trivial. For (2) the relation (2.15) follows from direct calculation of the partial trace. To check the commutation condition (2.12) we observe

$$[\mathbb{Q}_Q, \hat{\rho}_\beta \otimes \hat{\sigma}_{\beta\omega}] = \begin{pmatrix} 0 & e^{-\frac{\beta\omega}{2}} Q^* \hat{\rho}_\beta - e^{\frac{\beta\omega}{2}} \hat{\rho}_\beta Q^* \\ e^{\frac{\beta\omega}{2}} Q \hat{\rho}_\beta - e^{-\frac{\beta\omega}{2}} \hat{\rho}_\beta Q & 0 \end{pmatrix}$$

By Lemma 2.1 the relation $[Q, H] = \omega Q$ is equivalent to $e^{\beta\omega/2} \hat{\rho}_\beta Q = e^{-\beta\omega/2} Q \hat{\rho}_\beta$, so indeed the commutator vanishes. \blacksquare

As a last step we want to show that all Lindblad operator satisfying the DBC can be written in the form (2.11) with a particular choice of $\hat{\sigma}$, namely either $\hat{\sigma} = \hat{\rho}_\beta$ or $\hat{\sigma} = \hat{\rho}_\beta^{-1}$. Therefore, we introduce **partial transpose** on $L(\mathbf{H}_1 \otimes \mathbf{H}_2)$ that acts on the \mathbf{H}_2 part and is associated with a fixed $\hat{\sigma} = \hat{\sigma}^* > 0$, namely

$$\mathcal{T}_{\hat{\sigma}} : L(\mathbf{H}_1 \otimes \mathbf{H}_2) \rightarrow L(\mathbf{H}_1 \otimes \mathbf{H}_2) \text{ defined via } \mathcal{T}_{\hat{\sigma}}(A \otimes B) := A \otimes B^{\top_{\hat{\sigma}}} \quad (2.16)$$

and by linearity on $L(\mathbf{H}_1 \otimes \mathbf{H}_2)$. To define the $\hat{\sigma}$ -transpose $B^{\top_{\hat{\sigma}}}$ we write $\hat{\sigma} = \sum_{j=1}^J \sigma_j e_j \otimes \bar{e}_j$, where $\{e_j \in \mathbf{H}_2 \mid j = 1, \dots, J\}$ is an orthonormal basis in \mathbf{H}_2 , set $P_{jk} = e_j \otimes \bar{e}_k$, and let $P_{jk}^{\top_{\hat{\sigma}}} = P_{kj}$, which defines $B^{\top_{\hat{\sigma}}}$ by linearity. Clearly, $\mathcal{T}_{\hat{\sigma}}(\mathcal{T}_{\hat{\sigma}}\mathbb{Q}) = \mathbb{Q}$ and $\mathcal{T}_{\hat{\sigma}}\mathbb{Q}$ is Hermitian if and only if \mathbb{Q} is Hermitian.

Moreover, we define a $\hat{\sigma}$ -related operator $\mathbf{Y}_{\hat{\sigma}}$ from $L(\mathbf{H}_1 \otimes \mathbf{H}_2)$ into itself via

$$\mathbf{Y}_{\hat{\sigma}}\mathbb{Q} = (\mathbf{1}_{\mathbf{H}_1} \otimes \hat{\sigma}^{1/2}) (\mathcal{T}_{\hat{\sigma}}\mathbb{Q}) (\mathbf{1}_{\mathbf{H}_1} \otimes \hat{\sigma}^{1/2}), \quad (2.17)$$

With $P_{jk} = e_j \otimes \bar{e}_k$ from above, every $\mathbb{Q} \in L(\mathbf{H}_1 \otimes \mathbf{H}_2)$ has the unique representation $\mathbb{Q} = \sum_{j,k=1}^J Q_{jk} \otimes P_{jk}$, and we obtain the formulas

$$\mathcal{T}_{\hat{\sigma}}\mathbb{Q} = \sum_{j,k=1}^J Q_{kj} \otimes P_{jk} \quad \text{and} \quad \mathbf{Y}_{\hat{\sigma}}\mathbb{Q} = \sum_{j,k=1}^J \tilde{Q}_{jk} \otimes P_{jk} \quad \text{with} \quad \tilde{Q}_{jk} = (\sigma_j \sigma_k)^{1/2} Q_{kj}. \quad (2.18)$$

The following result show the interaction of the partial $\hat{\sigma}$ -transpose with commutators and the compact representation of Lindblad operators. In short, we show that a representation (2.11) for \mathcal{L} in terms of \mathbb{Q} and $\hat{\sigma}$ is equivalent to a representation in terms of $\mathbf{Y}_{\hat{\sigma}}\mathbb{Q}$ and $\hat{\sigma}^{-1}$.

Lemma 2.6 Consider $\hat{\sigma} \in L(\mathbf{H}_2)$ with $\hat{\sigma} = \hat{\sigma}^* > 0$. For $\mathbb{Q} \in L(\mathbf{H}_1) \otimes L(\mathbf{H}_2)$ we have

$$\mathcal{T}_{\hat{\sigma}}([\mathbb{Q}, A \otimes \hat{\sigma}]) = (\mathbf{1}_{\mathbf{H}_1} \otimes \hat{\sigma}^{1/2}) [\mathbf{Y}_{\hat{\sigma}} \mathbb{Q}, A \otimes \hat{\sigma}^{-1}] (\mathbf{1}_{\mathbf{H}_1} \otimes \hat{\sigma}^{1/2}) \quad \text{for all } A \in L(\mathbf{H}_1). \quad (2.19)$$

In particular, we have an equivalence between the commutation relations

$$[\mathbb{Q}, \hat{\rho}_{\beta} \otimes \hat{\sigma}] = 0 \quad \Longleftrightarrow \quad [\mathbf{Y}_{\hat{\sigma}} \mathbb{Q}, \hat{\rho}_{\beta} \otimes \hat{\sigma}^{-1}] = 0 \quad (2.20)$$

and the dual representations of the compact representation of Lindblad operators:

$$\text{Tr}_{\mathbf{H}_2} [\mathbb{Q}, [\mathbb{Q}, A \otimes \sigma]] = \text{Tr}_{\mathbf{H}_2} [\mathbf{Y}_{\hat{\sigma}} \mathbb{Q}, [\mathbf{Y}_{\hat{\sigma}} \mathbb{Q}, A \otimes \hat{\sigma}^{-1}]]. \quad (2.21)$$

Proof. To simplify notations we introduce $M_{\hat{\sigma}} := \mathbf{1}_{\mathbf{H}_1} \otimes \sigma^{1/2}$.

For establishing (2.19), we can use linearity such that it is sufficient to consider the case $\mathbb{Q} = Q_{kl} \otimes P_{lk}$, which gives

$$\mathcal{T}_{\hat{\sigma}}[\mathbb{Q}, A \otimes \hat{\sigma}] = \sigma_l(Q_{jk}A) \otimes P_{lk} - \sigma_k(AQ_{kl}) \otimes P_{lk}.$$

Moreover, using $\mathbf{Y}_{\hat{\sigma}} \mathbb{Q} = (\sigma_k \sigma_l)^{1/2} Q_{kl} \otimes P_{lk}$, we find

$$[\mathbf{Y}_{\hat{\sigma}} \mathbb{Q}, A \otimes \hat{\sigma}^{-1}] = (\sigma_l / \sigma_k)^{1/2} (Q_{kl}A) \otimes P_{lk} - (\sigma_k / \sigma_l)^{1/2} (AQ_{kl}) \otimes P_{lk}.$$

Since multiplying this expression from the left and from the right by $M_{\hat{\sigma}}$ reduces to multiplying by $(\sigma_k \sigma_l)^{1/2}$, we see that identity (2.19) is established.

Clearly, (2.20) follows from (2.19) by choosing $A = \hat{\rho}_{\beta}$ and using that $M_{\hat{\sigma}}$ is invertible.

Identity (2.21) follows by recalling the relation (2.13), which gives

$$-\text{Tr}_{\mathbf{H}_2} [\mathbb{Q}, [\mathbb{Q}, A \otimes \sigma]] = \sum_{k,l=1}^J \sigma_l ([Q_{kl}A, Q_{kl}^*] + [Q_{kl}, AQ_{kl}^*]).$$

Applying the same formula but with \mathbb{Q} and $\hat{\sigma}$ replaced by $\mathbf{Y}_{\hat{\sigma}} \mathbb{Q}$ and $\hat{\sigma}^{-1}$ we simply have to Q_{kl} by $Q_{kl} = (\sigma_k \sigma_l)^{1/2} Q_{lk}$ and the eigenvalues σ_l by $1/\sigma_l$. We then find the same result, and (2.21) is proved. \blacksquare

We now come to our representation of Lindblad operators satisfying the DBC with the choice $\hat{\sigma} = \hat{\rho}_{\beta}$ or $\hat{\sigma} = \hat{\rho}_{\beta}^{-1}$, which both are useful and have a natural interpretation. In the first case, we can use the fact for all $\rho \in \mathfrak{R} \subset L(\mathbf{H})$ the tensor product $\rho \otimes \hat{\rho}_{\beta}$ is again a density matrix, but now on the Hilbert space $\mathbf{H} \otimes \mathbf{H}$. In the second case the matrix $\rho \otimes \hat{\rho}_{\beta}^{-1}$ can be seen as a non-commutative counterpart of the relative density $\varrho(x) = u(x)/U^{\text{eq}}(x)$ in the Fokker-Planck equation or of the relative density $(p_n/w_n^{\text{eq}})_{n=1,\dots,N}$ for discrete Markov processes, see Section 3.1. Note also that the two commutation relations

$$[\mathbb{Q}, \hat{\rho}_{\beta} \otimes \hat{\rho}_{\beta}] = 0 \quad \text{and} \quad [\tilde{\mathbb{Q}}, \hat{\rho}_{\beta} \otimes \hat{\rho}_{\beta}^{-1}] = 0$$

look quite different, since $\hat{\rho}_{\beta} \otimes \hat{\rho}_{\beta}$ has the eigenvalues $\frac{1}{Z_{\beta}} e^{-\beta(\varepsilon_j + \varepsilon_k)}$ while $\hat{\rho}_{\beta} \otimes \hat{\rho}_{\beta}^{-1}$ has the eigenvalues $\frac{1}{Z_{\beta}} e^{-\beta(\varepsilon_j - \varepsilon_k)}$. So the latter appears closer to the relevant eigenpairs $(\omega, Q) \in \mathfrak{E}(H)$. However, we will see in the following proof, which is based on the previous lemma, that there is a one-to-one correspondence between all possible \mathbb{Q} and $\tilde{\mathbb{Q}}$.

Theorem 2.7 (Compact representation of \mathcal{L} with DBC) *Let \mathcal{L} be a Lindblad operator satisfying the DBC with respect to $\hat{\rho}_\beta \in L(\mathbf{H})$. Then, there exists a Hermitian $\mathbb{Q} \in L(\mathbf{H}) \otimes L(\mathbf{H}_1)$ satisfying the commutator relation $[\mathbb{Q}, \hat{\rho}_\beta \otimes \hat{\rho}_\beta] = 0$ such that the representation*

$$\mathcal{L}\rho = -\text{Tr}_{\mathbf{H}_2} \left([\mathbb{Q}, [\mathbb{Q}, \rho \otimes \hat{\rho}_\beta]] \right)$$

holds. Moreover, choosing $\tilde{\mathbb{Q}} = \mathbf{Y}_{\hat{\rho}_\beta} \mathbb{Q}$ as in Lemma 2.6, we have the alternative representation

$$\mathcal{L}\rho = -\text{Tr}_{\mathbf{H}_2} \left([\tilde{\mathbb{Q}}, [\tilde{\mathbb{Q}}, \rho \otimes \hat{\rho}_\beta^{-1}]] \right).$$

Proof. By [KF*77] every Lindblad operator satisfying detailed balance can be written in the form

$$\mathcal{L}(\rho) = \sum_{ij,mn} M_{ij,mn} ([P_{ij}\rho, P_{mn}^*] + [P_{ij}, \rho P_{mn}^*])$$

with $P_{ij} = h_i \otimes \bar{h}_j$, where h_i are the eigenvectors of $\hat{\rho}_\beta$, and $M_{ij,mn}$ satisfy

- (i) $\overline{M}_{mn,ij} = M_{ij,mn}$, (ii) $\varepsilon_j - \varepsilon_i \neq \varepsilon_n - \varepsilon_m \implies M_{ij,mn} = 0$,
- (iii) $M_{nm,ji} = e^{-\beta\omega} M_{ij,mn}$ with $\omega = \varepsilon_j - \varepsilon_i = \varepsilon_n - \varepsilon_m$.

We construct the Hermitian operator \mathbb{Q} in the form $\mathbb{Q} = \sum_{i,j,m,n} A_{ij,kl} P_{ij} \otimes P_{kl}^*$. Hence,

$$\begin{aligned} [\mathbb{Q}, \hat{\rho}_\beta \otimes \hat{\rho}_\beta] = 0 &\iff \left(A_{ij,kl} = 0 \text{ whenever } \varepsilon_j - \varepsilon_i \neq \varepsilon_l - \varepsilon_k \right), \\ \mathbb{Q}^* = \mathbb{Q} &\iff \overline{A}_{ij,kl} = A_{ji,lk}. \end{aligned}$$

To this end we define

$$\widetilde{M}_{ij,mn} = Z_\beta^2 e^{\beta(\varepsilon_i + \varepsilon_m)/2} M_{ij,mn}.$$

Then $\widetilde{M}_{ij,mn} = \widetilde{M}_{nm,ji} = \overline{\widetilde{M}_{ji,mn}}$. This symmetry property remains true for all powers of \widetilde{M} and thus for $\widetilde{M}^{\frac{1}{2}}$ as well. Define $A_{ij,kl} = e^{\beta \frac{\varepsilon_k - \varepsilon_i}{2}} (\widetilde{M}^{\frac{1}{2}})_{ij,kl}$. Then,

$$\begin{aligned} A_{ji,lk} &= e^{\beta \frac{\varepsilon_l - \varepsilon_j}{2}} (\widetilde{M}^{\frac{1}{2}})_{ji,lk} = e^{\beta \frac{\varepsilon_l - \varepsilon_j}{2}} \overline{(\widetilde{M}^{\frac{1}{2}})_{ij,kl}} \\ &= e^{\beta \frac{\varepsilon_l - \varepsilon_j}{2} - \beta \frac{\varepsilon_j - \varepsilon_i}{2}} \overline{A_{ij,kl}} = e^{\beta \frac{\omega - \omega}{2}} \overline{A_{ij,kl}} \end{aligned}$$

Thus the corresponding \mathbb{Q} is Hermitian and $A_{ij,kl} = 0$ if $\varepsilon_j - \varepsilon_i \neq \varepsilon_l - \varepsilon_k$ follows from condition (2) on $M_{ij,mn}$. Finally

$$\begin{aligned} \frac{1}{Z_\beta^2} \sum_{k,l} A_{ij,kl} \overline{A_{mn,kl}} e^{-\beta\varepsilon_k} &= \frac{1}{Z_\beta^2} \sum_{k,l} e^{\beta \frac{\varepsilon_k - \varepsilon_i}{2}} (\widetilde{M}^{\frac{1}{2}})_{ij,kl} \cdot e^{\beta \frac{\varepsilon_k - \varepsilon_m}{2}} \overline{(\widetilde{M}^{\frac{1}{2}})_{mn,kl}} e^{-\beta\varepsilon_k} \\ &= e^{-\beta \frac{\varepsilon_i + \varepsilon_m}{2}} \frac{1}{Z_\beta^2} \sum_{k,l} (\widetilde{M}^{\frac{1}{2}})_{ij,kl} (\widetilde{M}^{\frac{1}{2}})_{kl,mn} = e^{-\beta \frac{\varepsilon_i + \varepsilon_m}{2}} \frac{1}{Z_\beta^2} \widetilde{M}_{ij,mn} = H_{ij,mn} \end{aligned}$$

which means that

$$\mathcal{L}\rho = \sum_{ij,mn} M_{ij,mn} ([P_{ij}\rho, P_{mn}^*] + [P_{ij}, \rho P_{mn}^*]) = -\text{Tr}_{\mathbf{H}_2} \left([\mathbb{Q}, [\mathbb{Q}, \rho \otimes \hat{\rho}_\beta]] \right).$$

This establishes the first representation based on \mathbb{Q} and $\hat{\rho}_\beta$. The second representation involving $\tilde{\mathbb{Q}}_{\hat{\rho}_\beta}$ and $\hat{\rho}_\beta^{-1}$ follows simply by applying (2.21) to the case $\sigma = \hat{\rho}_\beta$. \blacksquare

2.4 Examples of Lindblad operators and equations

Here we give two elementary examples to highlight the structures and to come back to them in later sections.

2.4.1 The Bloch sphere for the case $N = 2$

For the case $\mathbf{H} = \mathbb{C}^2$ and $H = \text{diag}(\varepsilon_1, \varepsilon_2)$ with $\varepsilon_1 \neq \varepsilon_2$ we characterize all Lindblad operators \mathcal{L} on $\mathbb{C}_{\text{Herm}}^{2 \times 2}$ satisfying the DBC with respect to $\hat{\rho}_\beta$. For this we use the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

and the operators $\sigma_\pm = \frac{1}{2}(\sigma_1 \pm \sigma_2)$. Then, all \mathcal{L} have the form

$$\begin{aligned} \mathcal{L}_d(\rho) = & \frac{\gamma}{2} \left(e^{-\beta\varepsilon_1} ([\sigma_+\rho, \sigma_-] + [\sigma_+, \rho\sigma_-]) + e^{-\beta\varepsilon_2} ([\sigma_-\rho, \sigma_+] + [\sigma_-, \rho\sigma_+]) \right) \\ & + \frac{\delta}{2} ([\sigma_3\rho, \sigma_3] + [\sigma_3, \rho\sigma_3]), \end{aligned} \quad (2.22)$$

which are simply two building blocks with $Q = \sigma_+$, $Q^* = \sigma_-$, and $W = \sigma_3$.

It is more convenient to write the above generator in terms of real-valued Bloch coordinates $\mathbf{a} \in \mathbb{R}^3$ via $\rho(\mathbf{a}) = \frac{1}{2}\text{id} + \frac{1}{2}\sum_{i=1}^3 a_i \cdot \sigma_i$. The positivity $\rho \geq 0$ is equivalent to $|\mathbf{a}| \leq 1$. The Lindblad equation $\dot{\rho} = \mathcal{L}_d(\rho)$ reads $\dot{\mathbf{a}} = R\mathbf{a} + \mathbf{k}$ in Bloch coordinates with

$$R = \begin{pmatrix} -(\gamma+2\delta) & 0 & 0 \\ 0 & -(\gamma+2\delta) & 0 \\ 0 & 0 & -2\gamma \end{pmatrix}, \quad \mathbf{k} = \begin{pmatrix} 0 \\ 0 \\ 2\gamma\overline{w} \end{pmatrix} \quad (2.23)$$

with $\overline{w} = e^{-\beta\varepsilon_1} - e^{-\beta\varepsilon_2}$. This is the dissipative part of the well-known phenomenological Bloch equations. The longitudinal and transverse relaxation times T_1 and T_2 are given by $T_1 = \frac{1}{2\gamma}$ and $T_2 = \frac{1}{\gamma+2\delta}$. They satisfy the inequality $T_1 \geq \frac{1}{2}T_2$.

2.4.2 A nontrivial case

In this example we give a case where an eigenvalue $\omega \neq 0$ of $A \mapsto [A, H]$ is not simple, which allows for a nontrivial coupling between four energy levels.

In $\mathbf{H} = \mathbb{C}^4$ we choose $H = \sum_{i=1}^4 \varepsilon_i h_i$ with $\varepsilon_4 = 10$, $\varepsilon_3 = 9$, $\varepsilon_2 = 2$, $\varepsilon_1 = 1$, and $Q = h_1 \otimes \bar{h}_2 + h_3 \otimes \bar{h}_4$. Using $\varepsilon_4 - \varepsilon_3 = \varepsilon_2 - \varepsilon_1 = 1$ we have $(1, Q) \in \mathfrak{E}(H)$. Then, by Proposition 2.2(b) we see that

$$\dot{\rho} = \mathbf{M}_{\beta, Q} \rho = e^{\frac{\beta}{2}} ([QA, Q^*] + [Q, AQ^*]) + e^{-\frac{\beta}{2}} ([Q^*A, Q] + [Q^*, AQ]) \quad (2.24)$$

satisfies the DBC with respect to $\hat{\rho}_\beta$. Let us rewrite the above equation in coordinates. The diagonal elements form a Markov chain

$$\begin{aligned} \dot{\rho}_{11} &= -e^{-\frac{\beta}{2}} \rho_{11} + e^{\frac{\beta}{2}} \rho_{22} & \dot{\rho}_{33} &= -e^{-\frac{\beta}{2}} \rho_{33} + e^{\frac{\beta}{2}} \rho_{44} \\ \dot{\rho}_{22} &= +e^{-\frac{\beta}{2}} \rho_{11} - e^{\frac{\beta}{2}} \rho_{22} & \dot{\rho}_{44} &= +e^{-\frac{\beta}{2}} \rho_{33} - e^{\frac{\beta}{2}} \rho_{44} \end{aligned}$$

and the evolution of the off-diagonal elements is given by

$$\dot{\rho}_{13} = -e^{-\frac{\beta}{2}}\rho_{13} + e^{\frac{\beta}{2}}\rho_{24} \quad \dot{\rho}_{24} = +e^{-\frac{\beta}{2}}\rho_{13} - e^{\frac{\beta}{2}}\rho_{24}$$

and $\dot{\rho}_{kl} = -\cosh \frac{\beta}{2} \rho_{kl}$ for $(k, l) \notin \{(1, 3), (3, 1), (2, 4), (4, 2)\}$. This example shows, that non-diagonal elements (here ρ_{13} and ρ_{24}) can couple, if the energy differences are the same. Note that ρ_{11} and ρ_{22} are decoupled from ρ_{33} and ρ_{44} . Thus $\hat{\rho}_\beta$ is not the only equilibrium of (2.24). This is also the reason why ρ_{13} and ρ_{24} do not decay to 0, contrary to the other off-diagonal elements.

3 An entropic gradient structure for the Lindblad equation

3.1 Entropic gradient structures for classical Markov processes

The entropic gradient structure for master equations for classical Markov processes goes back to the seminal work [JKO97, JKO98], where the Fokker-Planck equation

$$\dot{u} = \operatorname{div} \left(a(x) (\nabla u + u \nabla V(x)) \right)$$

for the probability density $u(t, x) \geq 0$ was written as a gradient system with respect to the Wasserstein distance. Here $a(x) \in \mathbb{R}^{d \times d}$ is a symmetric and positive definite diffusion matrix. The gradient structure namely in the form

$$\dot{u} = -\mathbb{K}_W(u) D\mathcal{F}(u),$$

where \mathcal{F} is the free energy (or relative entropy with respect to the equilibrium density $U^{\text{eq}}(x) = e^{-V(x)}$) and \mathbb{K}_W is the Onsager operator associated with the Wasserstein distance, namely

$$\begin{aligned} \mathcal{F}(u) &= \int_{\mathbb{R}^d} \left(u(x) \log u(x) + V(x)u(x) \right) dx = \int_{\mathbb{R}^d} u(x) \log (u(x)/U^{\text{eq}}(x)) dx, \\ \mathbb{K}_W(u)\xi &= -\operatorname{div} (u a(x) \nabla \xi) \end{aligned}$$

A related gradient structure for time-continuous Markov processes on a discrete state space $\{1, \dots, N\}$ was found independently by the three groups [Maa11, ErM12], [CH*12], and [Mie11b, Mie13b]. In this case the Kolmogorov forward equation (also called master equation) for the probability vector $p(t) \in \{ (p_1, \dots, p_N) \in [0, 1]^N \mid \sum_{n=1}^N p_n = 1 \}$ is the simply linear system

$$\dot{p} = Lp, \quad \text{where } L_{nm} \geq 0 \text{ for } n \neq m \text{ and } L^\top(1, 1, \dots, 1)^\top = 0.$$

The detailed balance condition for L and the equilibrium w^{eq} reads

$$Lw^{\text{eq}} = 0 \text{ with } w_n^{\text{eq}} > 0 \quad \text{and} \quad \kappa_{nm} := L_{nm}w_m^{\text{eq}} = L_{mn}w_n^{\text{eq}} \text{ for all } n, m \in \{1, \dots, N\}.$$

The entropic gradient structure is defined in term of the relative entropy $\mathcal{E}(p) = \mathcal{H}(p|w^{\text{eq}})$ and the Onsager operator $\mathbb{K}_M(p)$ with

$$\mathcal{E}(p) = \sum_{n=1}^N p_n \log(p_n/w_n^{\text{eq}}) \text{ and } \mathbb{K}_M(p) = \sum_{m>n} \kappa_{nm} \Lambda\left(\frac{p_n}{w_n^{\text{eq}}}, \frac{p_m}{w_m^{\text{eq}}}\right) (e_n - e_m) \otimes (e_n - e_m),$$

where $\Lambda(a, b) \geq 0$ denotes the *logarithmic mean of a and b*:

$$\Lambda(a, b) = \int_0^1 a^s b^{1-s} ds = \frac{a - b}{\log a - \log b}. \quad (3.1)$$

Note that using $D\mathcal{E}(p) = (\log p_n - \log w_n^{\text{eq}})_{n=1, \dots, N}$, the relation $\Lambda(a, b)(\log a - \log b) = a - b$, and the detailed balance condition easily yield the identity $Lp = -\mathbb{K}_M(p)D\mathcal{E}(p)$.

3.2 The Kubo-Mori operator \mathfrak{C}_ρ and the generalization \mathfrak{D}_ρ^α

The development of an analogous gradient structure for the dissipative part of the Lindblad equation as a gradient system was less successful. The attempts in [Ött10, Ött11, Mie13a, Mie15] produced nonlinear terms, unless the Hamiltonian H is a multiple of $\mathbf{1}_H$ (as in [CaM14] or more generally only the building blocks \mathbf{S}_W in Proposition 2.2 are used). All of these works involve the Kubo-Mori operator $\mathfrak{C}_\rho : L(\mathbf{H}) \rightarrow L(\mathbf{H})$ as a generalization of the multiplication with u in the Fokker-Planck equation and the logarithmic mean $\Lambda(\frac{p_n}{w_n^{\text{eq}}}, \frac{p_m}{w_m^{\text{eq}}})$. It is defined via

$$\mathfrak{C}_\rho A := \int_0^1 \rho^s A \rho^{1-s} ds = \sum_{n,m=1}^N \Lambda(r_n, r_m) \langle \psi_n | A \psi_m \rangle \psi_n \otimes \bar{\psi}_m,$$

if ρ is given by (2.2).

One major property of \mathfrak{C}_ρ is that it satisfies the analog of the identities

$$u \nabla \log(u/e^{-V}) = \nabla u + u \nabla V \quad \text{and} \quad \Lambda(a, b)(\log a - \log b) = a - b \quad (3.2)$$

for the classical Markov setting. Note that the right-hand sides are linear in u and (a, b) , respectively. For all $Q \in L(\mathbf{H})$ the operator \mathfrak{C}_ρ satisfies a similar “miracle identity”, namely

$$\mathfrak{C}_\rho[Q, \log \rho] = [Q, \rho], \quad (3.3)$$

see [Ött10, Ött11, Mie13a, Mie15]. We will provide a proof of a more general version of this identity in Proposition 3.1.

This relation works well (see [CaM14]) if we are using the total entropy $\mathcal{S}_0(\rho) = -\text{Tr}(\rho \log \rho)$ which has the derivative $D\mathcal{S}(\rho) = -\log \rho$ (up to an identity which is irrelevant since $\text{Tr} \rho = 1$). However, for relative entropies of the form $\mathcal{S}_\beta(\rho) = -\text{Tr}(\beta H \rho + \rho \log \rho)$ we have

$$D\mathcal{S}_\beta(\rho) = -\beta H - \log \rho \quad \rightsquigarrow \quad \mathfrak{C}_\rho[Q, D\mathcal{S}_\beta(\rho)] = -[Q, \rho] - \mathfrak{C}_\rho[Q, H].$$

Thus, the right-hand side is no longer linear, unless Q commutes with H . The Fokker-Planck equation studied in [CaM14] has $H = 0$ and hence falls into this class, i.e. the

Fokker-Planck equation is indeed a linear Lindblad equation. However, the models studied in [Ött10, Ött11, Mie13a, Mie15] include the nonsmooth term $\mathfrak{C}_\rho[Q, H]$, which is continuous but not Hölder continuous, so the existence theory developed in [Mie13a, Sec. 21.6] is nontrivial and uniqueness of solutions couldn't be established.

We now show that it is possible to use variants of \mathfrak{C}_ρ such that for $(\omega, Q) \in \mathfrak{E}(H)$ we obtain a suitable counterpart of (3.2). Indeed we will be able to show that all Lindblad operators satisfying detailed balance can be written in terms of these variants of \mathfrak{C}_ρ . The variant of \mathfrak{C}_ρ we are using is defined in terms of the tilted operator \mathfrak{D}_ρ^α , where $\alpha \in \mathbb{R}$ will relate to an energy difference:

$$\mathfrak{D}_\rho^\alpha A := e^{-\alpha/2} \int_0^1 e^{s\alpha} \rho^s A \rho^{1-s} ds = \sum_{n,k=1}^N \Lambda(e^{\alpha/2} r_n, e^{-\alpha/2} r_k) \langle \psi_n | A | \psi_k \rangle \psi_n \otimes \bar{\psi}_k, \quad (3.4)$$

if ρ is given by (2.2). Again the logarithmic mean $\Lambda(a, b)$ from (3.1) is involved, but now weighted by $e^{\pm\alpha/2}$.

The generalized miracle identity is given in the following result (3.7), which again shows that applying \mathfrak{D}_ρ^α to a commutator with $\log \rho$ plus a suitable correction provides a linear expression, i.e. the nonlinearities involved in $\log \rho$ and \mathfrak{D}_ρ^α cancel each other.

Proposition 3.1 *For all $\alpha \in \mathbb{R}$, $A, Q \in \mathbb{C}^{N \times N}$, and $\rho \in \mathfrak{R}_>$ we have the identities*

$$(\mathfrak{D}_\rho^\alpha)^* = \mathfrak{D}_\rho^\alpha \quad \text{and} \quad (\mathfrak{D}_\rho^\alpha A^*)^* = \mathfrak{D}_\rho^{-\alpha} A, \quad (3.5)$$

$$\langle A | \mathfrak{D}_\rho^\alpha A \rangle \geq 0, \quad (3.6)$$

$$\mathfrak{D}_\rho^\alpha([Q, \log \rho] - \alpha Q) = e^{-\alpha/2} Q \rho - e^{\alpha/2} \rho Q. \quad (3.7)$$

Proof. The relations in (3.5) follow directly from the definition. For (3.6) we use

$$\begin{aligned} \langle A | \mathfrak{D}_\rho^\alpha A \rangle &= e^{-\alpha/2} \int_0^1 e^{s\alpha} \langle A | \rho^s A \rho^{1-s} \rangle ds \\ &= \int_0^1 e^{\alpha(s-1/2)} \text{Tr}((\rho^{s/2} A \rho^{s/2})^* \rho^{s/2} A \rho^{s/2} \rho^{1-2s}) ds \geq 0, \end{aligned}$$

since the integrand is non-negative for all $s \in [0, 1]$.

For (3.7), we generalize the simple proof of (3.3) from [Mie13a, Prop. 21.1], write $\Lambda = \log \rho$, and use the fact that the integrand defining \mathfrak{D}_ρ^α can be written as a total derivative with respect to $s \in [0, 1]$:

$$\begin{aligned} \mathfrak{D}_\rho^\alpha([Q, \log \rho] - \alpha Q) &= e^{-\alpha/2} \int_0^1 e^{\alpha s} e^{s\Lambda} (Q\Lambda - \Lambda Q - \alpha\Lambda) e^{(1-s)\Lambda} ds \\ &= -e^{-\alpha/2} \int_0^1 \left(e^{\alpha s} e^{s\Lambda} (\Lambda + \alpha I) Q e^{(1-s)\Lambda} + e^{\alpha s} e^{s\Lambda} Q (-\Lambda) e^{(1-s)\Lambda} \right) ds \\ &= -e^{-\alpha/2} \int_0^1 \frac{d}{ds} \left(e^{(\Lambda + \alpha I)s} Q e^{(1-s)\Lambda} \right) ds = e^{-\alpha/2} (Q e^\Lambda - e^{\Lambda + \alpha I} Q) \\ &= e^{-\alpha/2} Q \rho - e^{\alpha/2} \rho Q. \end{aligned}$$

This is the desired result. \blacksquare

The following result follows immediately from the above proposition by setting $\alpha = -\beta\omega$. It will be the basis for our construction of the entropic gradient structure.

Corollary 3.2 *Assume $\beta > 0$ and that $(\omega, H) \in \mathfrak{E}(H)$, that is $[Q, H] = \omega Q$, then*

$$\mathfrak{D}_\rho^{-\beta\omega} [Q, \log \rho + \beta H] = e^{\beta\omega/2} Q \rho - e^{-\beta\omega/2} \rho Q. \quad (3.8)$$

The next lemma shows that \mathfrak{D}_ρ^α appears naturally if we tensorize ρ with a diagonal matrix, and thus connects our construction with that in Section 2.3.

Lemma 3.3 *For all $\rho \in \mathfrak{R}$ and all $\alpha \in \mathbb{R}$ we have*

$$\mathfrak{C} \begin{pmatrix} e^{\alpha/2} \rho & 0 \\ 0 & e^{-\alpha/2} \rho \end{pmatrix} \begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} e^{\alpha/2} \mathfrak{C}_\rho A & \mathfrak{D}_\rho^\alpha B \\ \mathfrak{D}_\rho^{-\alpha} C & e^{-\alpha/2} \mathfrak{C}_\rho D \end{pmatrix}.$$

Proof. This follows simply using the identity (for $a, b > 0$)

$$\begin{pmatrix} a\rho & 0 \\ 0 & b\rho \end{pmatrix}^s = \begin{pmatrix} a^s \rho^s & 0 \\ 0 & b^s \rho^s \end{pmatrix}$$

and the definitions of $\mathfrak{C}_{\begin{pmatrix} \rho_1 & 0 \\ 0 & \rho_2 \end{pmatrix}}$ and \mathfrak{D}_ρ^α from above. \blacksquare

As was pointed out in Section 2.3 every Lindblad operator can be written as the sum of partial traces of double commutators on a larger tensor product space. This enlarged space also has the advantage, that the miracle identity (3.7) becomes very elegant and more transparent, when taking the original miracle identity for granted.

Theorem 3.4 (Generalized miracle identity) *Let $\mathbb{Q} \in L(\mathbf{H}_1 \otimes \mathbf{H}_2)$, $\hat{\rho} \in L(\mathbf{H}_1)$, and $\hat{\sigma} \in L(\mathbf{H}_2)$ satisfy $\hat{\rho} = \hat{\rho}^* > 0$, $\hat{\sigma} = \hat{\sigma}^* > 0$, and the commutator relation (2.12), i.e. $[\mathbb{Q}, \hat{\rho}_\beta \otimes \hat{\sigma}] = 0$. Then, for all $\rho \in \mathfrak{R}$ we have the identity*

$$\mathfrak{C}_{\rho \otimes \hat{\sigma}} [\mathbb{Q}, (\log \rho - \log \hat{\rho}_\beta) \otimes \mathbf{1}_{\mathbf{H}_2}] = [\mathbb{Q}, \rho \otimes \hat{\sigma}]. \quad (3.9)$$

Proof. Using Lemma 2.4 in “ $\stackrel{*}{=}$ ” below we obtain the following chain of identities:

$$\begin{aligned} \mathfrak{C}_{\rho \otimes \hat{\sigma}} [\mathbb{Q}, (\log \rho - \log \hat{\rho}) \otimes \mathbf{1}_{\mathbf{H}_2}] &= \mathfrak{C}_{\rho \otimes \hat{\sigma}} [\mathbb{Q}, (\log \rho) \otimes \mathbf{1}_{\mathbf{H}_2}] - \mathfrak{C}_{\rho \otimes \hat{\sigma}} [\mathbb{Q}, (\log \hat{\rho}) \otimes \mathbf{1}_{\mathbf{H}_2}] \\ &\stackrel{*}{=} \mathfrak{C}_{\rho \otimes \hat{\sigma}} [\mathbb{Q}, (\log \rho) \otimes \mathbf{1}_{\mathbf{H}_2}] + \mathfrak{C}_{\rho \otimes \hat{\sigma}} [\mathbb{Q}, \mathbf{1}_{\mathbf{H}_1} \otimes (\log \hat{\sigma})] \\ &= \mathfrak{C}_{\rho \otimes \hat{\sigma}} [\mathbb{Q}, (\log \rho) \otimes \mathbf{1}_{\mathbf{H}_2} + \mathbf{1}_{\mathbf{H}_1} \otimes (\log \hat{\sigma})] = \mathfrak{C}_{\rho \otimes \hat{\sigma}} [\mathbb{Q}, \log(\rho \otimes \hat{\sigma})] \stackrel{\circ}{=} [\mathbb{Q}, \rho \otimes \hat{\sigma}], \end{aligned}$$

where “ $\stackrel{\circ}{=}$ ” uses the classical miracle identity (3.3). \blacksquare

We note that relation (3.8) in Corollary 3.2 is a direct consequence of Theorem 3.4 by setting

$$\mathbb{Q} = \begin{pmatrix} 0 & Q^* \\ Q & 0 \end{pmatrix} \quad \hat{\sigma} = \begin{pmatrix} e^{\beta\omega/2} & 0 \\ 0 & e^{-\beta\omega/2} \end{pmatrix}.$$

3.3 Dissipation potential and Onsager operator

We now complete the task of writing the dissipative part \mathcal{L} of any Lindblad operator satisfying the DBC with respect to $\hat{\rho}_\beta$ as a gradient of the relative entropy, namely

$$\mathcal{F}(\rho) = \mathcal{H}(\rho|\hat{\rho}_\beta) := \text{Tr} \left(\rho (\log \rho - \log \hat{\rho}_\beta) \right) = \text{Tr} (\rho \log \rho + \rho \beta H) + \log Z_\beta.$$

The aim is to construct an Onsager operator $\mathbb{K}(\rho)$ such that

$$\mathcal{L}\rho = -\mathbb{K}(\rho)D\mathcal{F}(\rho) = -\mathbb{K}(\rho)(\log \rho + \beta H).$$

The symmetric and positive definite Onsager operator $\mathbb{K}(\rho)$ is most easily defined in terms of a non-negative and quadratic dual dissipation potential

$$\mathcal{R}^*(\rho, \xi) = \frac{1}{2} \langle \xi | \mathbb{K}(\rho) \xi \rangle.$$

Such structure is most easily obtained by using the compact tensor product formulation for Lindblad operators \mathcal{L} developed in Section 2.3, namely

$$\mathcal{L}\rho = -\text{Tr}_{H_2} \left([\mathbb{Q}, [\mathbb{Q}, \rho \otimes \hat{\sigma}]] \right). \quad (3.10)$$

This will also give corresponding gradient structure when \mathcal{L} is given by the building blocks of Proposition 2.2, namely

$$\mathcal{L}\rho = \sum_{j=1}^J \mathbf{M}_{\beta, Q_j} \rho \quad \text{where } (\omega_j, Q_j) \in \mathfrak{E}(H).$$

Indeed, each building block can be expressed in tensor form with $\hat{\sigma}_j = 1$ or $\hat{\sigma}_n \in \mathbb{R}^{2 \times 2}$. If we construct a suitable $\mathbf{K}_j(\rho)$ for each of the building blocks, we can use the additivity principle for Onsager operators, i.e. the sum $\mathbb{K}(\rho) := \sum_{j=1}^J \mathbf{K}_j(\rho)$ is the desired total Onsager operator.

Indeed, the tensorial representation (3.10) for Lindblad operators satisfying the DBC with respect to $\hat{\rho}_\beta$, the commutator relation $[\mathbb{Q}, \hat{\rho}_\beta \otimes \hat{\sigma}] = 0$, and the tensorial miracle identity (3.9) leads us to the following general result.

Proposition 3.5 (Onsager operators and dissipation potentials) *For given \mathbb{Q} , $\hat{\rho}_\beta$, and $\hat{\sigma}$ that satisfy the commutation relation $[\mathbb{Q}, \hat{\rho}_\beta \otimes \hat{\sigma}] = 0$, we define the Onsager operator $\mathbb{K} : \mathbb{C}_{\text{Herm}}^{N \otimes N} \rightarrow \mathbb{C}_{\text{Herm}}^{N \otimes N}$ and the dual dissipation potential $\mathcal{R}^* : \mathbb{C}_{\text{Herm}}^{N \otimes N} \rightarrow \mathbb{R}$ via*

$$\begin{aligned} \mathbb{K}(\rho)\xi &:= \text{Tr}_{H_2} \left([\mathbb{Q}, \mathfrak{C}_{\rho \otimes \hat{\sigma}}[\mathbb{Q}, \xi \otimes \mathbf{1}_{H_2}]] \right) \\ \mathcal{R}^*(\rho, \xi) &:= \frac{1}{2} \left\langle [\mathbb{Q}, \xi \otimes \mathbf{1}_{H_2}], \mathfrak{C}_{\rho \otimes \hat{\sigma}}[\mathbb{Q}, \xi \otimes \mathbf{1}_{H_2}] \right\rangle. \end{aligned}$$

Then,

$$\mathbb{K}(\rho)(\log \rho - \log \hat{\rho}_\beta) = \text{Tr}_{H_2}([\mathbb{Q}, [\mathbb{Q}, \rho \otimes \hat{\sigma}]] \quad (3.11)$$

as well as

$$\mathbb{K}(\rho) = \mathbb{K}(\rho)^* \geq 0, \quad \mathbb{K}(\rho)\xi = D_\xi \mathcal{R}^*(\rho, \xi), \quad \langle \xi, \mathbb{K}(\rho)\xi \rangle = 2\mathcal{R}^*(\rho, \xi) \geq 0.$$

Proof. We first observe that relation (3.11) follows by employing Theorem 3.4. The positivity of \mathcal{R}^* is a special case of Proposition 3.1 for $\alpha = 0$, i.e. $\mathfrak{C}_{\rho \otimes \hat{\sigma}} \geq 0$. Finally, we obtain $\mathbb{K}(\rho)\xi = D_\xi \mathcal{R}^*(\rho, \xi)$ by noting that Tr_{H_2} is adjoint to $A \mapsto A \otimes \mathbf{1}_{H_2}$. This then shows $\mathbb{K} = \mathbb{K}^* \geq 0$. ■

Note that the operators \mathbb{Q} and $\hat{\sigma}$ strongly depend on H and β since they have to satisfy the commutation relation $[\mathbb{Q}, \hat{\rho}_\beta \otimes \hat{\sigma}] = 0$. The relation (3.11) shows that the above gradient structure does indeed lead to Lindblad operators satisfying detailed balance. A direct corollary of the above gradient structure are the Onsager operators for the building blocks $\mathbf{M}_{\beta, Q}$ introduced in Proposition 2.2.

Corollary 3.6 (Simple Onsager operators) *Given H and $\hat{\rho}_\beta$ as above and $(\omega, Q) \in \mathfrak{E}(H)$, we define $\mathbf{K}_{\beta, Q}(\rho) : \mathbb{C}_{\text{Herm}}^{N \times N} \rightarrow \mathbb{C}_{\text{Herm}}^{N \times N}$ and $\mathcal{R}_{\beta, Q}^* : \mathbb{C}_{\text{Herm}}^{N \times N} \rightarrow [0, \infty[$ as follows:*

$$\mathbf{K}_{\beta, Q}(\rho)\xi := [Q^*, [\mathfrak{D}_\rho^{-\beta\omega}[Q, \xi]]] + [Q, [\mathfrak{D}_\rho^{\beta\omega}[Q^*, \xi]]]$$

Then $\mathbf{K}_{\beta, Q}$ is an Onsager operator as in Proposition 3.5 and satisfies the identity

$$\mathbf{M}_{\beta, Q}\rho = -\mathbf{K}_{\beta, Q}(\rho)(\log \rho + \beta H) \quad (3.12)$$

Proof. Choose

$$\mathbb{Q} = \begin{pmatrix} 0 & Q^* \\ Q & 0 \end{pmatrix} \quad \hat{\sigma} = \begin{pmatrix} e^{\beta\omega/2} & 0 \\ 0 & e^{-\beta\omega/2} \end{pmatrix}.$$

Then equation (3.12) follows directly from (3.11) and Lemma 3.3. ■

Our main result concerning the representation of general Lindblad operators satisfying a DBC is now simply stated by collecting the previous results. We have two forms, the first is based on the compact tensor representation and the second is based on the additive form $\mathcal{L} = \sum_{m=1}^M \mathbf{M}_{\beta, Q_m}$ in terms of the building blocks \mathbf{M}_{β, Q_m} , which will be reflected in an additive structure for the Onsager operator \mathbb{K} , whereas the relative entropy as the driving functional is independent of the M different dissipative mechanisms.

Theorem 3.7 (Gradient structure for \mathcal{L} with DBC) *Consider $\beta > 0$, $H \in \mathbb{C}_{\text{Herm}}^{N \times N}$, and $\hat{\rho}_\beta$ as above. Then, for any Lindblad operator \mathcal{L} satisfying the DBC (2.5) there exists an Onsager operator \mathbb{K} such that \mathcal{L} can be written as \mathbb{K} -gradient of the relative entropy $\mathcal{F}_\beta = \mathcal{H}(\cdot | \hat{\rho}_\beta)$.*

(1) If $\mathcal{L}\rho = -\text{Tr}_{H_2}([\mathbb{Q}, [\mathbb{Q}, \rho \otimes \hat{\rho}_\beta]]) = -\text{Tr}_{H_2}([\tilde{\mathbb{Q}}, [\tilde{\mathbb{Q}}, \rho \otimes \hat{\rho}_\beta^{-1}]])$ with $\tilde{\mathbb{Q}} = \mathbf{Y}_{\hat{\rho}_\beta} \mathbb{Q}$, we can choose

$$\mathbb{K}(\rho)\xi = \text{Tr}_{H_2}([\mathbb{Q}, \mathfrak{C}_{\rho \otimes \hat{\rho}_\beta}[\mathbb{Q}, \xi \otimes \mathbf{1}_{H_2}]]) = \text{Tr}_{H_2}([\tilde{\mathbb{Q}}, \mathfrak{C}_{\rho \otimes \hat{\rho}_\beta^{-1}}[\tilde{\mathbb{Q}}, \xi \otimes \mathbf{1}_{H_2}]])$$

(2) If $\mathcal{L} = \sum_{m=1}^M \mathbf{M}_{\beta, Q_m}$ with $(\omega_m, Q_m) \in \mathfrak{E}(H)$, we can choose $\mathbb{K}(\rho) = \sum_{m=1}^M \mathbf{K}_{\beta, Q_m}(\rho)$.

Proof. The result (1) follows by combining the tensor representation in Theorem 2.7 and Proposition 3.5. The result (2) follows by combining the additive representation in Proposition 2.2(c) and Corollary 3.6. ■

4 Dissipative quantum mechanics via GENERIC

GENERIC is an acronym for General Equations for Non-Equilibrium Reversible Irreversible Coupling, which was introduced by Öttinger and Grmela in [GrÖ97, ÖtG97]. It described a thermodynamic consistent way of coupling Hamiltonian (=reversible) dynamics with gradient-flow (irreversible) dynamics. It is a variant of metriplectic systems introduced in [Mor84, Mor86], see also [Mor09]. We refer to [MiT14] for an introductory survey of this framework and applications in a large variety of applications. After our general introduction in Section 4.1 we will mainly dwell on the quantum mechanical papers [Ött10, Ött11, Mie13a].

4.1 General setup of GENERIC

A GENERIC system is defined in terms of a quintuple $(\mathbf{Q}, \mathcal{E}, \mathcal{S}, \mathbb{J}, \mathbb{K})$, where the smooth functionals \mathcal{E} and \mathcal{S} on the state space \mathbf{Q} denote the total energy and the total entropy, respectively. Moreover, \mathbf{Q} carries two geometric structure, namely a Poisson structure \mathbb{J} and a dissipative structure \mathbb{K} , i.e., for each $q \in \mathbf{Q}$ the operators $\mathbb{J}(q)$ and $\mathbb{K}(q)$ map the cotangent space $T_q^*\mathbf{Q}$ into the tangent space $T_q\mathbf{Q}$. The evolution of the system is given by the differential equation

$$\dot{q} = \mathbb{J}(q)D\mathcal{E}(q) + \mathbb{K}(q)D\mathcal{S}(q), \quad (4.1)$$

where $D\mathcal{E}$ and $D\mathcal{S}$ are the differentials taking values in the cotangent space.

The basic conditions on the geometric structures \mathbb{J} and \mathbb{K} are the symmetries

$$\mathbb{J}(q) = -\mathbb{J}(q)^* \quad \text{and} \quad \mathbb{K}(q) = \mathbb{K}(q)^* \quad (4.2a)$$

and the structural properties

$$\begin{aligned} \mathbb{J} \text{ satisfies Jacobi's identity,} \\ \mathbb{K}(q) \text{ is positive semi-definite, i.e., } \langle \xi, \mathbb{K}(q)\xi \rangle \geq 0. \end{aligned} \quad (4.2b)$$

Thus, the triples $(\mathbf{Q}, \mathcal{E}, \mathbb{J})$ and $(\mathbf{Q}, \mathcal{S}, \mathbb{K})$ form a Hamiltonian and an Onsager or gradient system, respectively, with evolution equations $\dot{q} = \mathbb{J}(q)D\mathcal{E}(q)$ and $\dot{q} = \mathbb{K}(q)D\mathcal{S}(q)$, respectively. Finally, the central condition states that the energy functional does not contribute to dissipative mechanisms and that the entropy functional does not contribute to reversible dynamics, which is the following ***non-interaction condition (NIC)***:

$$\forall q \in \mathbf{Q} : \quad \mathbb{J}(q)D\mathcal{S}(q) = 0 \quad \text{and} \quad \mathbb{K}(q)D\mathcal{E}(q) = 0. \quad (4.2c)$$

A first observation is that (4.2) implies energy conservation and entropy increase:

$$\frac{d}{dt}\mathcal{E}(q(t)) = \langle D\mathcal{E}(q), \dot{q} \rangle = \langle D\mathcal{E}(q), \mathbb{J}D\mathcal{E} + \mathbb{K}D\mathcal{S} \rangle = 0 + 0 = 0, \quad (4.3)$$

$$\frac{d}{dt}\mathcal{S}(q(t)) = \langle D\mathcal{S}(q), \dot{q} \rangle = \langle D\mathcal{S}(q), \mathbb{J}D\mathcal{E} + \mathbb{K}D\mathcal{S} \rangle = 0 + \langle D\mathcal{S}, \mathbb{K}D\mathcal{S} \rangle \geq 0. \quad (4.4)$$

Note that we would need much less than the three conditions (4.2) to guarantee these two properties. However, the next property needs (4.2c) in its full strength.

Next, we show that equilibria can be obtained by the *maximum entropy principle*. If x_{eq} maximizes \mathcal{S} under the constraint $\mathcal{E}(q) = E_0$, then we obtain a Lagrange multiplier $\lambda_{\text{eq}} \in \mathbb{R}$ such that $\text{D}\mathcal{S}(q_{\text{eq}}) = \lambda_{\text{eq}} \text{D}\mathcal{E}(q_{\text{eq}})$. Assuming $\lambda_{\text{eq}} \neq 0$ we immediately find that x_{eq} is an equilibrium of (4.1). Indeed,

$$\mathbb{J}(q_{\text{eq}})\text{D}\mathcal{E}(q_{\text{eq}}) = \frac{1}{\lambda_{\text{eq}}}\mathbb{J}(q_{\text{eq}})\text{D}\mathcal{S}(q_{\text{eq}}) = 0 \text{ and } \mathbb{K}(q_{\text{eq}})\text{D}\mathcal{S}(q_{\text{eq}}) = \lambda_{\text{eq}}\mathbb{K}(q_{\text{eq}})\text{D}\mathcal{E}(q_{\text{eq}}) = 0,$$

where we used the NIC (4.2c).

Vice versa, for every steady state q_{eq} of (4.1) we must have

$$\mathbb{J}(q_{\text{eq}})\text{D}\mathcal{E}(q_{\text{eq}}) = 0 \text{ and } \mathbb{K}(q_{\text{eq}})\text{D}\mathcal{S}(q_{\text{eq}}) = 0. \quad (4.5)$$

Thus, in a steady state there cannot be any balancing between reversible and irreversible forces, both have to vanish independently. To see this we simply recall the entropy production relation (4.4), which implies $\langle \text{D}\mathcal{S}(q_{\text{eq}}), \mathbb{K}(q_{\text{eq}})\text{D}\mathcal{S}(q_{\text{eq}}) \rangle = 0$ for any steady state. Since $\mathbb{K}(q_{\text{eq}})$ is positive semidefinite, this implies the second identity in (4.5). The first identity then follows from $\dot{q} \equiv 0$ in (4.1).

Very often one is only interested in isothermal systems with fixed temperature $\theta_* > 0$, where the free energy $\mathcal{F}(q) = \mathcal{E}(q) - \theta_*\mathcal{S}(q)$ is a Liapunov function. The associated structure is then that of a damped Hamiltonian system, namely

$$\dot{q} = \left(\mathbb{J}(q) - \frac{1}{\theta_*}\mathbb{K}(q) \right) \text{D}\mathcal{F}(q), \quad (4.6)$$

where again \mathbb{J} and \mathbb{K} are Poisson and Onsager structures, respectively. However, there are no longer any non-interaction conditions, since only one functional \mathcal{F} is left.

As in [Mie11a, DPZ13] we note that (4.6) can be converted to a GENERIC system by introducing a scalar slack variable e and defining $wt\mathcal{E}(q, e) = \mathcal{F}(q) + e$, $\tilde{\mathcal{S}}(q, e) = \frac{e}{\theta_*}$,

$$\tilde{\mathbb{J}}(q, e) = \begin{pmatrix} \mathbb{J}(q) & 0 \\ 0 & 0 \end{pmatrix}, \quad \text{and} \quad \tilde{\mathbb{K}}(q, e) = \begin{pmatrix} \mathbb{K} & -\mathbb{K}\text{D}\mathcal{F} \\ -(\mathbb{K}\text{D}\mathcal{F})^\top & \langle \text{D}\mathcal{F}, \mathbb{K}\text{D}\mathcal{F} \rangle \end{pmatrix}.$$

Clearly, the NIC (4.2c) are satisfied. The variable e can be seen as the entropic part of the energy. Of course, in concrete cases it is usually easy to find a physically more reasonable splitting into entropy and energy.

4.2 Coupling a dissipative and a quantum system

Since GENERIC systems are closed systems with energy conservation and entropy increase, we need to model all couplings to the quantum system by suitable macroscopic variables. For this aim we introduce the macroscopic variables z lying in a Hilbert space Z . The macro-variable z may include Hamiltonian parts (like the Maxwell equations) as well as dissipative parts producing entropy. The important point of this work is the thermodynamically consistent coupling of the macroscopic system to the quantum system in such a way that energy can be exchanged via Lindblad-like terms.

Following [Ött10, Ött11, Mie13a] we consider an energy and an entropy in the decoupled form

$$\mathcal{E}(\rho, z) = \text{Tr}(\rho H) + E(z) \quad \text{and} \quad \mathcal{S}(\rho, z) = -k_B \text{Tr}(\rho \log \rho) + S(z). \quad (4.7)$$

Whenever suitable we abbreviate the full state with $q = (\rho, z)$ and choose a Poisson structure as follows. Consider a constant macroscopic Poisson operator $\mathbb{J}_{\text{ma}}(z) : Z^* \rightarrow Z$ and a constant coupling operator $\Gamma : \mathbb{C}^{N \times N} \rightarrow Z$, then

$$\mathbb{J}(q) = \begin{pmatrix} \mathbb{J}_{\text{qs}}(\rho) & -\mathbb{J}_{\text{qs}}(\rho)\Gamma^* \\ -\Gamma\mathbb{J}_{\text{qs}}(\rho) & \mathbb{J}_{\text{ma}} + \Gamma\mathbb{J}_{\text{qs}}(\rho)\Gamma^* \end{pmatrix} \text{ with } \mathbb{J}_{\text{qs}}(\rho)\mu = \text{i}[\rho, \mu], \quad (4.8)$$

is a Poisson structure, which easily follows by transforming the decoupled structure $\text{diag}(\mathbb{J}_{\text{qs}}, \mathbb{J}_{\text{ma}})$ via the linear mapping $(\rho, z) \mapsto (\rho, z - \Gamma\rho)$.

Using the relation $\text{D}\mathcal{S}(q) = (-k_{\text{B}} \log \rho, \text{D}_z S(z))$ and $[\rho, \log \rho] = 0$, the NIC $\mathbb{J}(q)\text{D}\mathcal{S}(q) \equiv 0$ follows by asking

$$\mathbb{J}_{\text{ma}}(z)\text{D}_z S(z) \equiv 0 \quad \text{and} \quad \Gamma^* \text{D}_z S(z) \equiv 0. \quad (4.9)$$

The choice for the Onsager operator \mathbb{K} is more delicate, since we do not want to generate nonlinear (non-smooth) terms arising from $-k_{\text{B}} \log \rho$ in the term $\mathbb{K}(q)\text{D}\mathcal{S}(q)$. This will be achieved by using the theory from above concerning the gradient structures for the Lindblad equation for a fixed quantum Hamiltonian H and coupling operators Q_c , where $c \in C$ is a finite set of couplings. Throughout we assume that $(\omega_c, Q_c) \in \mathfrak{E}(H)$ are fixed, while the inverse coupling temperatures $\beta_c(z)$ may depend on the state of the macroscopic system.

More precisely, for the dual entropy-production potential of the coupled system we use the ansatz

$$\begin{aligned} \mathcal{P}^*(\rho, z; \mu, \zeta) &= \frac{1}{2} \langle \zeta, \mathbb{K}_{\text{ma}}(z)\zeta \rangle_Z \\ &+ \sum_{c \in C} \frac{1}{2} \langle \mu - \langle \zeta, b_c(z) \rangle H \mid \widehat{\mathbb{K}}_c(z) (\mu - \langle \zeta, b_c(z) \rangle H) \rangle. \end{aligned} \quad (4.10)$$

Here $\mathbb{K}_{\text{ma}}(z) : Z^* \rightarrow Z$ is a symmetric and positive semi-definite macroscopic Onsager operator. The coupling vectors $b_c(z) \in Z$ are chosen to satisfy the conditions

$$\forall c \in C \quad \forall z \in Z : \quad \langle \text{D}_z E(z), b_c(z) \rangle_Z = 1 \text{ and } \langle \text{D}_z S(z), b_c(z) \rangle_Z > 0. \quad (4.11)$$

where the first ensures the NIC $\mathbb{K}(\rho, z)\text{D}\mathcal{E}(\rho, z) \equiv 0$ and the second the positivity of the temperature. The Onsager operators $\widehat{\mathbb{K}}_c(z)$ are chosen using our operators $\mathbf{K}_{\beta, Q}(\rho) : \mathbb{C}^{N \times N} \rightarrow \mathbb{C}^{N \times N}$ from Corollary 3.6 as follows:

$$\widehat{\mathbb{K}}_c(z) = \kappa_c(z) \mathbf{K}_{\widehat{\beta}_c(z), Q_c}(\rho), \quad \text{where } \widehat{\beta}_c(z) := \frac{1}{k_{\text{B}}} \langle \text{D}_z S(z), b_c(z) \rangle_Z \text{ and } \kappa_c(z) \geq 0. \quad (4.12)$$

Hence, the full Onsager operator takes the form

$$\mathbb{K}(q) = \begin{pmatrix} 0 & 0 \\ 0 & \mathbb{K}_{\text{ma}}(z) \end{pmatrix} + \sum_{c \in C} \begin{pmatrix} \widehat{\mathbb{K}}_c & -\langle \square, b_c \rangle_Z \widehat{\mathbb{K}}_c H \\ -\langle H \mid \widehat{\mathbb{K}}_c \square \rangle b_c & \langle H \mid \widehat{\mathbb{K}}_c H \rangle b_c \otimes b_c \end{pmatrix}, \quad (4.13)$$

where \square is the placeholder where the corresponding argument has to be inserted. Using the definition of $\widehat{\beta}_c$ in (4.12) we easily see that the NIC $\mathbb{K}(\rho, z)\text{D}\mathcal{E}(\rho, z) \equiv 0$ holds, if we assume $\mathbb{K}_{\text{ma}}(z)\text{D}_z E(z) \equiv 0$. We emphasize that \mathbb{K} does depend highly nonlinearly on ρ through $\mathbf{K}_{\beta_c(z), H}(\rho)$, which in turn depends on $\mathfrak{D}_{\rho}^{\pm \widehat{\beta}_c(z) \omega_c}$.

Proposition 4.1 (GENERIC structure) *Let $X = \mathfrak{R} \times Z$ and let \mathcal{E} and \mathcal{S} be given in the decoupled form (4.7). Moreover, consider the Poisson structure \mathbb{J} defined in (4.8) and the Onsager structure \mathbb{K} defined in (4.13). Assuming additionally (4.11), $\mathbb{J}_{\text{ma}}\text{DS} \equiv 0$, $\Gamma^*\text{DS} \equiv 0$, and $\mathbb{K}_{\text{ma}}\text{DE} \equiv 0$ the quintuple $(X, \mathcal{E}, \mathcal{S}, \mathbb{J}, \mathbb{K})$ forms a GENERIC system.*

So far, we have not used the special form of $\widehat{\mathbb{K}}_c$ defined in terms of $\mathbf{K}_{\beta_c, Q_c}$. The advantage of this choice is of course dictated by the aim to obtain a linear Lindblad equation for ρ . Indeed, using the relation (3.12) relating $\mathbf{K}_{\beta, Q}$ and $\mathbf{M}_{\beta, Q}$ we see that the equations obtained from the GENERIC system have the explicit form

$$\begin{aligned} \begin{pmatrix} \dot{\rho} \\ \dot{z} \end{pmatrix} &= \mathbb{J}(\rho, z)\text{D}\mathcal{E}(\rho, z) + \mathbb{K}(\rho, z)\text{D}\mathcal{S}(\rho, z) \\ &= \begin{pmatrix} \mathbb{J}_{\text{qs}}(\rho) & -\mathbb{J}_{\text{qs}}(\rho)\Gamma^* \\ -\Gamma\mathbb{J}_{\text{qs}}(\rho) & \mathbb{J}_{\text{ma}} + \Gamma\mathbb{J}_{\text{qs}}(\rho)\Gamma^* \end{pmatrix} \begin{pmatrix} H \\ \text{DE}(z) \end{pmatrix} + \begin{pmatrix} 0 \\ \mathbb{K}_{\text{ma}}(z)\text{DS}(z) \end{pmatrix} \\ &\quad + \sum_{c \in C} \begin{pmatrix} \widehat{\mathbb{K}}_c & -\langle \square, b_c \rangle_Z \widehat{\mathbb{K}}_c H \\ -\langle H | \widehat{\mathbb{K}}_c \square \rangle_{b_c} & \langle H | \widehat{\mathbb{K}}_c H \rangle_{b_c \otimes b_c} \end{pmatrix} \begin{pmatrix} -k_B \log \rho \\ \text{DS}(z) \end{pmatrix}. \end{aligned} \quad (4.14)$$

Introducing the effective Hamiltonian $\widetilde{H}(z)$, which depends on the macroscopic z , by

$$\widetilde{H}(z) = H - \Gamma^*\text{DE}(z).$$

and using the construction of $\widehat{\mathbb{K}}_c(\rho, z)$ via $\mathbf{K}_{\widehat{\beta}_c(z), Q_c}(\rho)$ we arrive at a coupled system for ρ and z that is indeed linear in ρ , namely

$$\begin{aligned} \begin{pmatrix} \dot{\rho} \\ \dot{z} \end{pmatrix} &= \begin{pmatrix} i[\rho, \widetilde{H}(z)] \\ \mathbb{J}_{\text{ma}}\text{DE}(z) - i\Gamma[\rho, \widetilde{H}(z)] \end{pmatrix} + \begin{pmatrix} 0 \\ \mathbb{K}_{\text{ma}}(z)\text{DS}(z) \end{pmatrix} \\ &\quad + \sum_{c \in C} \begin{pmatrix} k_B \kappa_c(z) \mathbf{M}_{\beta_c(z), Q_c} \rho \\ -k_B \kappa_c(z) \langle H | \mathbf{M}_{\beta_c(z), Q_c} \rho \rangle_{b_c(z)} \end{pmatrix}. \end{aligned} \quad (4.15)$$

Moreover, the coupling of the linear quantum system for ρ with the macroscopic system for z is given in a very particular manner.

We emphasize the fact that this equation is obtained from the GENERIC system $(\mathfrak{R} \times Z, \mathcal{E}, \mathcal{S}, \mathbb{J}, \mathbb{K})$, so we know that we have energy conservation and entropy production along solutions $q(t) = (\rho(t), z(t))$, namely $\frac{d}{dt}\mathcal{E}(q(t)) \equiv 0$ and

$$\begin{aligned} \frac{d}{dt}\mathcal{S}(q(t)) &= 2\mathcal{P}^*(q(t), \text{DS}(t)) \\ &= 2\langle \text{DS}, \mathbb{K}_{\text{ma}}\text{DS} \rangle_Z + 2k_B^2 \sum_{c \in C} \langle \log \rho + \widehat{\beta}_c H | \mathbf{K}_{\widehat{\beta}_c, Q_c}(\log \rho + \widehat{\beta}_c H) \rangle \geq 0. \end{aligned}$$

For these relations to be true it was essential to choose $\widehat{\mathbb{K}}_c$ and hence $\mathbf{K}_{\beta, Q}$ in a very particular way. Moreover, it was crucial to normalize $b_c(z)$ and $\widehat{\beta}_c(z)$ in such a way that

$$\langle \text{DE}(z), b_c(z) \rangle_Z = 1 \quad \text{and} \quad \langle \text{DS}(z), b_c(z) \rangle_Z = k_B \widehat{\beta}_c(z),$$

see (4.11) and (4.12).

5 Examples and applications

We discuss the above construction and give a few examples and applications to highlight the concept of the operators \mathfrak{D}_ρ^α and the relevance of the corresponding Lindblad operators. From a modeling point of view we expect that dissipative mechanics in the macroscopic system and in the quantum system are given building blocks that have to be combined in a suitable way to obtain thermodynamically correct system, either a GENERIC system or a damped Hamiltonian system.

5.1 The isothermal, damped quantum system

For a general Lindblad operator \mathcal{L} satisfying the detailed balance condition (DBC) (2.5) with respect to $\hat{\rho}_\beta = \frac{1}{Z}e^{-\beta H}$ we have shown in Proposition 2.2 that it can be written in terms of operators $\mathbf{M}_{\beta,Q}$. Indeed, we have

$$\dot{\rho} = i[\rho, H] + \mathcal{L}\rho = i[\rho, H] + \sum_{c \in C} \mathbf{M}_{\beta, Q_c} \rho, \quad (5.1)$$

where $\mathbf{M}_{\beta, Q}$ is defined in Proposition 2.2(b) and each coupling operator Q_c satisfies $(\omega_c, Q_c) \in \mathfrak{E}(H)$.

We are now able to state that all dissipative quantum generators satisfying the DBC can be written as a damped Hamiltonian system $(\mathfrak{R}, \mathcal{F}, \mathbb{J}, \mathbb{K})$, namely

$$\dot{\rho} = i[\rho, H] + \mathcal{L}\rho = (\mathbb{J}_{\text{qs}}(\rho) - \mathbb{K}(\rho)) D\mathcal{F}(\rho),$$

where we can use the following choices

$$\mathcal{F}(\rho) = \text{Tr}(\beta H + \rho \log \rho), \quad \mathbb{J}_{\text{qs}}(\rho) = i[\rho, \square], \quad \text{and} \quad \mathbb{K}(\rho) = \sum_{c \in C} \mathcal{K}_{\beta, Q_c}(\rho).$$

For this we simply use that $(\omega, Q) \in \mathfrak{E}(H)$ implies the relation $\mathbf{K}_{\beta, Q}(\log \rho + \beta H) = \mathbf{M}_{\beta, Q} \rho$, see (3.12).

5.2 Coupling to simple heat baths

We consider a quantum system coupled to a finite number of finite-energy heat baths indexed by $m = 1, \dots, M$. We set $Z = \mathbb{R}^M$ with elements $z = \boldsymbol{\theta} = (\theta_m)_m$, where $\theta_m > 0$ denotes the absolute temperature of the m th heat bath. We assume each heat bath to have a constant specific heat c_m . Hence, we let

$$E(\boldsymbol{\theta}) = \sum_{m=1}^M c_m \theta_m \quad \text{and} \quad S(\boldsymbol{\theta}) = \sum_{m=1}^M c_m \log \theta_m.$$

For the coupling vectors b_m we choose

$$b_m(\boldsymbol{\theta}) = \frac{1}{c_m} \mathbf{e}^{(m)} \in \mathbb{R}^M, \quad \text{where } \mathbf{e}^{(m)} = (0, \dots, 0, 1, 0, \dots, 0)^\top$$

is the m th unit vector. Clearly we find

$$b_m(\boldsymbol{\theta}) \cdot DE(\boldsymbol{\theta}) \equiv 1 \quad \text{and} \quad \widehat{\beta}_m(\boldsymbol{\theta}) = \frac{1}{k_B} b_m(\boldsymbol{\theta}) \cdot DS(\boldsymbol{\theta}) = \frac{1}{k_B \theta_m},$$

which is the usual inverse temperature of the m th heat bath.

Assuming $\mathbb{J}_{\text{ma}} \equiv 0$ and $\Gamma = 0$, we can choose a symmetric and positive semi-definite matrix $K_{\text{ma}} \in \mathbb{R}^{M \times M}$ such that $K_{\text{ma}} \bar{\mathbf{c}} = 0$, where $\bar{\mathbf{c}}$ is the constant vector $DE(\boldsymbol{\theta}) = (1/c_m)_{m=1,\dots,M}$ the construction in Section 4.2 provides a GENERIC system for $q = (\rho, \boldsymbol{\theta})$ in the following form:

$$\begin{aligned} \dot{\rho} &= i[\rho, H] + \sum_{m=1}^M \mathbf{M}_{1/(k_B \theta_m), Q_m} \rho, \\ \dot{\boldsymbol{\theta}} &= K_{\text{ma}} DS(\boldsymbol{\theta}) + \sum_{m=1}^M \frac{1}{c_m} \langle H \mid \mathbf{M}_{1/(k_B \theta_m), Q_m} \rho \rangle \mathbf{e}^{(m)}. \end{aligned} \tag{5.2}$$

It is now easy to see that we may take the heat capacities very large, such that the temperatures θ_m do not change any more, or at least not on the time scale where the typical changes of ρ occur. Thus, it is possible to investigate in a natural way non-equilibrium steady states where energy is exchanged between heat baths with different temperatures.

5.3 An isothermally coupled system

Here we again consider an isothermally system where the quantum states are coupled to a macroscopic variable in such a way that we obtain a damped Hamiltonian system. In contrast to the simple model in Section 5.1 we now allow the effective inverse temperatures $\widehat{\beta}_c$ to depend on the state z . However, for the definition of the free energy \mathcal{F} we choose the fixed equilibrium temperature, namely

$$\mathcal{F}(\rho, z) = \frac{1}{k_B \theta_*} \mathcal{E}(\rho, z) - \frac{1}{k_B} \mathcal{S}(\rho, z) = \text{Tr}(\rho \log \rho + \beta_* \rho H) + F(z).$$

We may take \mathbb{J} as in (4.8) but need to choose a special \mathbb{K} to obtain equations linear in ρ , namely

$$\mathbb{K}(\rho, z) = \begin{pmatrix} 0 & 0 \\ 0 & \mathbb{K}_{\text{ma}}(z) \end{pmatrix} + \sum_{c \in C} \begin{pmatrix} \widetilde{\mathbb{K}}_c & \langle \square, a_c \rangle_Z \widetilde{\mathbb{K}}_c H \\ \langle H \mid \widetilde{\mathbb{K}}_c \square \rangle_{a_c} & \langle H \mid \widetilde{\mathbb{K}}_c H \rangle_{a_c \otimes a_c} \end{pmatrix}$$

with operators $\widetilde{\mathbb{K}}_c(\rho, z) = \kappa_c(z) \mathbf{K}_{\widetilde{\beta}_c(z), Q_c}(\rho)$, where

$$\kappa_c(z) \geq 0 \quad \text{and} \quad \widetilde{\beta}_c(z) = \beta_* + \langle DF(z), a_c(z) \rangle_Z > 0.$$

Hence, the equations $\dot{q} = (\mathbb{J}(q) - \mathbb{K}(q)) D\mathcal{F}(q)$ take the form

$$\begin{aligned} \dot{\rho} &= i[\rho, H - \Gamma^* DF(z)] + \sum_{c \in C} \kappa_c(z) \mathbf{M}_{\widetilde{\beta}_c(z), Q_c} \rho, \\ \dot{z} &= \mathbb{J}_{\text{ma}} DF(z) - i\Gamma[\rho, H - \Gamma^* DF(z)] + \sum_{c \in C} \kappa_c(z) \langle H \mid \mathbf{M}_{\widetilde{\beta}_c(z), Q_c} \rho \rangle a_c(z). \end{aligned}$$

Again we emphasize that $F(Z)$, $a_c(z)$, and $\tilde{\beta}_c(z)$ must be intrinsically linked to each other in order to generate this system by the damped Hamiltonian system $(\mathfrak{R} \times Z, \mathcal{F}, \mathbb{J}, \mathbb{K})$.

5.4 Maxwell-Bloch model

In this section we discuss a nonlinear PDE model, where the Maxwell equations on \mathbb{R}^3 as the macroscopic Hamiltonian system are coupled to a spatially localized domain $\Omega \subset \mathbb{R}^3$, where at each macroscopic point $x \in \Omega$ there is a quantum system that is coupled to the electromagnetic fields \mathbf{E} and \mathbf{H} , but not to the neighboring quantum systems. Such models are called Maxwell-Bloch systems (cf. e.g. [JMR00, Dum05]) and are commonly used to model the interaction of light and matter. We refer to [Mie15] where even the coupling to the drift-diffusion system for electrons and holes is described in terms of the GENERIC framework.

The macroscopic system is described by $z = (\mathbf{E}, \mathbf{H}) \in Z := L^2(\mathbb{R}^3; \mathbb{R}^3)^2$ denoting the electric and the magnetic fields. The optically active material is described by a bounded Lipschitz domain $\Omega \subset \mathbb{R}^3$, where the quantum state is described via $\rho : \Omega \rightarrow \mathfrak{R}_N \subset \mathbb{C}_{\text{Herm}}^{N \times N}$. The quantum state determines the macroscopic polarization $\mathbf{P} : \Omega \rightarrow \mathbb{R}^3$ via a polarization operator $\Gamma : \mathbb{C}^{N \times N} \rightarrow \mathbb{R}^3$ in the form $\mathbf{P}(x) = \Gamma \rho(x)$. The electric displacement field then is given by $\mathbf{D} = \varepsilon_0 \mathbf{E} + \mathbf{P}$, and Maxwell equations take the form

$$\varepsilon_0 \dot{\mathbf{E}} + \dot{\mathbf{P}} = \text{curl } \mathbf{H}, \quad \mu_0 \dot{\mathbf{H}} = -\text{curl } \mathbf{E}, \quad \text{div}(\varepsilon_0 \mathbf{E} + \mathbf{P}) = 0, \quad \text{div } \mathbf{H} = 0. \quad (5.3)$$

The main difficulty is to model the coupling of the quantum systems $\rho(t, x) \in \mathfrak{R}_N$ in a consistent way. We derive the system for $q := (\rho, \mathbf{E}, \mathbf{H})$ in the form of a damped Hamiltonian system with the free energy

$$\mathcal{F}(q) = \int_{\mathbb{R}^d} \frac{1}{2} |\mathbf{E}|^2 + \frac{1}{2} |\mathbf{H}|^2 dx + \int_{\Omega} \text{Tr}(\rho \log \rho + \beta H_B \rho) dx,$$

where H_B is called the Bloch Hamiltonian and where we have set the constants ε_0 and μ_0 to 1 for notational simplicity. Moreover, we define a Poisson structure \mathbb{J} and an Onsager operator \mathbb{K} in the form

$$\mathbb{J}(q) = \begin{pmatrix} i[\rho, \square] & -i[\rho, \Gamma^* \square] & 0 \\ -i\Gamma[\rho, \square] & i\Gamma[\rho, \Gamma^* \square] & \text{curl} \\ 0 & -\text{curl} & 0 \end{pmatrix} \quad \text{and} \quad \mathbb{K}(q) = \begin{pmatrix} \mathbb{K}_{\text{qs}}(q) & -\mathbb{K}_{\text{qs}}(q)\Gamma^* & 0 \\ -\Gamma\mathbb{K}_{\text{qs}}(q) & \Gamma\mathbb{K}_{\text{qs}}(q)\Gamma^* & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

The importance of this choice for \mathbb{J} and \mathbb{K} is that the first row of each of the block operators is replicated in the second row, but premultiplied with $-\Gamma$. This is needed to obtain the correct first equation in the Maxwell system (5.3), namely

$$\dot{\mathbf{E}} = \text{curl } \mathbf{H} - \dot{\mathbf{P}} = \text{curl } \mathbf{H} - \Gamma \dot{\rho}.$$

By the symmetries $\mathbb{J} = -\mathbb{J}^*$ and $\mathbb{K} = \mathbb{K}^*$ this also implies that the first columns are replicated in the second columns, but now post-multiplied by $-\Gamma^*$.

We emphasize that the optically active material is restricted to the bounded domain Ω , while the fields \mathbf{E} and \mathbf{H} are defined on all of \mathbb{R}^3 . This is hidden in our operator

Γ , which should be understood as an operator that maps ρ defined on Ω to vector fields $\mathbf{P} = \Gamma\rho$ that are defined not only in Ω , but that are extended by 0 outside of Ω . Similarly, the adjoint operator Γ^* acts on \mathbf{E} by restricting it first to Ω and then applying the adjoint map of Γ .

Thus, using $[\rho, \log \rho] = 0$ the induced equation for ρ reads

$$\dot{\rho} = i[\rho, \beta H_B - \Gamma^* \mathbf{E}] - \mathbb{K}_{\text{qs}}(\rho, \mathbf{E}, \mathbf{H})(\log \rho + \beta H_B - \Gamma^* \mathbf{E}).$$

Having derived this structure it is now our task to choose \mathbb{K}_{qs} in such a way that the equation for ρ is a Lindblad equation that is linear in ρ with coefficients depending on \mathbf{E} and \mathbf{H} . For this, we assume that there exists a family $(Q_c)_{c \in C}$ of couplings such that

$$(\omega_c, Q_c) \in \mathfrak{E}(H_B) \quad \text{and} \quad [Q_c, \Gamma^* \mathbf{E}] = \omega_c(\mathbf{g}_c \cdot \mathbf{E}) Q_c, \quad (5.4)$$

for some vectors $\mathbf{g}_c \in \mathbb{R}^3$. Note that this is a non-trivial condition, since it implies that for all $\mathbf{E} \in \mathbb{R}^3$ the matrix $\Gamma^* \mathbf{E} \in \mathbb{C}_{\text{Herm}}^{N \times N}$ commutes with all matrices Q that commute with H .

Based on the assumption (5.4) we are now able to choose \mathbb{K}_{qs} in the form

$$\mathbb{K}_{\text{qs}}(\rho, \mathbf{E}, \mathbf{H}) = \sum_{c \in C} \kappa_c(\mathbf{E}, \mathbf{H}) \mathbf{K}_{\tilde{\beta}_c(\mathbf{E}), Q_c}(\rho), \quad \text{where } \tilde{\beta}_c(\mathbf{E}) := \beta - \mathbf{g}_c \cdot \mathbf{E}.$$

Since by construction we have $[Q_c, \beta H_B - \Gamma^* \mathbf{E}] = \omega_c \tilde{\beta}_c(\mathbf{E}) Q_c$ we can apply Proposition 3.6 (cf. (3.12)) and obtain the equation

$$\dot{\rho} = i[\rho, \beta H_B - \Gamma^* \mathbf{E}] + \sum_{c \in C} \kappa_c(\mathbf{E}, \mathbf{H}) \mathbf{M}_{\tilde{\beta}_c(\mathbf{E}), Q_c} \rho,$$

which is linear in ρ for fixed \mathbf{E} and \mathbf{H} . Note that for the above constructions it is not necessary to have $\tilde{\beta}_c \geq 0$, since $\mathbf{K}_{\beta, Q}$ and $\mathbf{M}_{\beta, Q}$ are well defined for all $\beta \in \mathbb{R}$.

Altogether the damped Hamiltonian system $(L^2(\Omega; \mathfrak{R}_N) \times Z, \mathcal{F}, \mathbb{J}, \mathbb{K})$ generates the coupled system

$$\begin{aligned} \dot{\rho} &= i[\rho, H_B - \Gamma^* \mathbf{E}] + \sum_{c \in C} \kappa_c(q) \mathbf{M}_{\beta, Q_c} \rho, \\ \dot{\mathbf{E}} &= \text{curl } \mathbf{H} - \Gamma \left(i[\rho, H_B - \Gamma^* \mathbf{E}] + \sum_{c \in C} \kappa_c(q) \mathbf{M}_{\beta, Q_c} \rho \right), \\ \dot{\mathbf{H}} &= -\text{curl } \mathbf{E}. \end{aligned}$$

References

- [Ali76] R. ALICKI. On the detailed balance condition for non-Hamiltonian systems. *Rep. Math. Phys.*, 10(2), 249–258, 1976.
- [CaM14] E. A. CARLEN and J. MAAS. An analog of the 2-Wasserstein metric in non-commutative probability under which the fermionic Fokker–Planck equation is gradient flow for the entropy. *Commun. Math. Phys.*, 331(3), 887–926, 2014.
- [CH*12] S.-N. CHOW, W. HUANG, Y. LI, and H. ZHOU. Fokker-Planck equations for a free energy functional or Markov process on a graph. *Arch. Rational Mech. Anal.*, 203(3), 969–1008, 2012.

- [Dav74] E. B. DAVIES. Markovian master equations. *Comm. Math. Phys.*, 39, 91–110, 1974.
- [DPZ13] M. H. DUONG, M. A. PELETIER, and J. ZIMMER. GENERIC formalism of a Vlasov-Fokker-Planck equation and connection to large-deviation principles. *Nonlinearity*, 26(11), 2951–2971, 2013.
- [Dum05] É. DUMAS. Global existence for Maxwell-Bloch systems. *J. Diff. Eqns.*, 219(2), 484–509, 2005.
- [ErM12] M. ERBAR and J. MAAS. Ricci curvature of finite Markov chains via convexity of the entropy. *Arch. Rational Mech. Anal.*, 206(3), 997–1038, 2012.
- [GrÖ97] M. GRMELA and H. C. ÖTTINGER. Dynamics and thermodynamics of complex fluids. I. Development of a general formalism. *Phys. Rev. E (3)*, 56(6), 6620–6632, 1997.
- [JKO97] R. JORDAN, D. KINDERLEHRER, and F. OTTO. Free energy and the fokker-planck equation. *Physica D*, 107(2-4), 265–271, 1997.
- [JKO98] R. JORDAN, D. KINDERLEHRER, and F. OTTO. The variational formulation of the Fokker-Planck equation. *SIAM J. Math. Analysis*, 29(1), 1–17, 1998.
- [JMR00] J.-L. JOLY, G. METIVIER, and J. RAUCH. Transparent nonlinear geometric optics and Maxwell-Bloch equations. *J. Differential Equations*, 166(1), 175–250, 2000.
- [KF*77] A. KOSSAKOWSKI, A. FRIGERIO, V. GORINI, and M. VERRI. Quantum detailed balance and KMS condition. *Comm. Math. Phys.*, 57(2), 97–110, 1977.
- [Maa11] J. MAAS. Gradient flows of the entropy for finite Markov chains. *J. Funct. Anal.*, 261, 2250–2292, 2011.
- [Mie11a] A. MIELKE. Formulation of thermoelastic dissipative material behavior using GENERIC. *Contin. Mech. Thermodyn.*, 23(3), 233–256, 2011.
- [Mie11b] A. MIELKE. A gradient structure for reaction-diffusion systems and for energy-drift-diffusion systems. *Nonlinearity*, 24, 1329–1346, 2011.
- [Mie13a] A. MIELKE. Dissipative quantum mechanics using GENERIC. In A. Johann, H.-P. Kruse, F. Rupp, and S. Schmitz, editors, *Recent Trends in Dynamical Systems*, pages 555–586. Springer Verlag, 2013. Proceedings of a Conference in Honor of Jürgen Scheurle.
- [Mie13b] A. MIELKE. Geodesic convexity of the relative entropy in reversible Markov chains. *Calc. Var. Part. Diff. Eqns.*, 48(1), 1–31, 2013.
- [Mie15] A. MIELKE. On thermodynamical couplings of quantum mechanics and macroscopic systems. In P. Exner, W. König, and H. Neidhardt, editors, *Mathematical Results in Quantum Mechanics*, pages 331–348, Singapore, 2015. World Scientific. Proceedings of the QMath12 Conference.
- [MiT14] A. MIELKE and M. THOMAS. GENERIC — a powerful tool for thermomechanical modeling. *In preparation*, 2014.
- [Mor84] P. J. MORRISON. Bracket formulation for irreversible classical fields. *Phys. Lett. A*, 100(8), 423–427, 1984.
- [Mor86] P. J. MORRISON. A paradigm for joined Hamiltonian and dissipative systems. *Phys. D*, 18(1-3), 410–419, 1986.
- [Mor09] P. J. MORRISON. Thoughts on brackets and dissipation: old and new. *J. Physics: Conf. Series*, 169, 012006, 12, 2009.
- [Ons31] L. ONSAGER. Reciprocal relations in irreversible processes, I+II. *Physical Review*, 37, 405–426, 1931. (part II, 38:2265–2279).
- [ÖtG97] H. C. ÖTTINGER and M. GRMELA. Dynamics and thermodynamics of complex fluids. II. Illustrations of a general formalism. *Phys. Rev. E (3)*, 56(6), 6633–6655, 1997.
- [Ött10] H. C. ÖTTINGER. The nonlinear thermodynamic quantum master equation. *Phys. Rev. A*, 82, 052119(11), 2010.
- [Ött11] H. C. ÖTTINGER. The geometry and thermodynamics of dissipative quantum systems. *Europhys. Lett.*, 94, 10006(6), 2011.
- [Spo78] H. SPOHN. Entropy production for quantum dynamical semigroups. *J. Mathematical Phys.*, 19(5), 1227–1230, 1978.